

STATIONARITY, TIME-REVERSAL AND FLUCTUATION THEORY FOR A CLASS OF PIECEWISE DETERMINISTIC MARKOV PROCESSES

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ABSTRACT. We consider a class of stochastic dynamical systems, called piecewise deterministic Markov processes, with states $(x, \sigma) \in \Omega \times \Gamma$, Ω being a region in \mathbb{R}^d or the d -dimensional torus, Γ being a finite set. The continuous variable x follows a piecewise deterministic dynamics, the discrete variable σ evolves by a stochastic jump dynamics and the two resulting evolutions are fully-coupled. We study stationarity, reversibility and time-reversal symmetries of the process. Increasing the frequency of the σ -jumps, we show that the system behaves asymptotically as deterministic and we investigate the structure of fluctuations (i.e. deviations from the asymptotic behavior), recovering in a non Markovian frame results obtained by Bertini et al. [1, 2, 3, 4], in the context of Markovian stochastic interacting particle systems. Finally, we discuss a Gallavotti-Cohen-type symmetry relation with involution map different from time-reversal. For several examples the above results are recovered by explicit computations.

Key words: Non-equilibrium Processes, Large Deviations, Stationary States.

1. INTRODUCTION

Piecewise deterministic Markov processes (PDMPs) are stochastic dynamical systems whose state is described by a pair (x, σ) , where x is a continuous variable and σ is a discrete variable. We take $x \in \Omega$ and $\sigma \in \Gamma$, Ω being a region in \mathbb{R}^d or the d -dimensional torus, Γ being a finite set. Motivated by applications to biochemical processes [13], we call x and σ the mechanical and the chemical variable (or state) of the system, respectively. The chemical state σ evolves by a random jump dynamics, while in the intervals in which the chemical state is kept constant and equal to some σ , the mechanical state x evolves according to the deterministic σ -dependent ODE $\dot{x}(t) = F_\sigma(x(t))$. Since the probability rates of chemical jumps can depend on x , the mechanical state x and the chemical one σ are dynamically fully-coupled. In our analysis, we restrict to time-homogeneous PDMPs, i.e. both the vector fields $F_\sigma(x)$ and the probability rate $\lambda r(\sigma, \sigma' | x)$ for a chemical jump from σ to σ' at the x -mechanical state are time-independent. Above, λ is a positive parameter we will play with in order to analyze some special regime. The above models can be used to describe the overdamped motion of a particle in a viscous fluid under alternating force fields, as well as some biochemical processes as discussed in [13]

PDMPs are broadly used in applied sciences and engineering, and are a typical example of what is called a *stochastic hybrid system* in control theory [8]. A mathematical analysis of PDMPs has been started by Davies in [9] and the interested reader can find a detailed mathematical treatment in [10]. Our interest here is mainly theoretical and inspired by the physics of out-of-equilibrium systems. In particular, our investigation concerns the steady state, the time-reversed process, the deviations of the system from its typical behavior, a

special fluctuation–dissipation relation and a Gallavotti–Cohen–type symmetry relation. We discuss our results in more detail.

In general, under mixing assumptions, the steady state (stationary measure) is unique and has density $\rho_\lambda(x, \sigma)$ on $\Omega \times \Gamma$ which solves a system of differential equations with zero–flux boundary conditions. We give exact solutions in dimension one, while for any dimension we isolate a class of exactly solvable models for which ρ_λ has the special form

$$\rho_\lambda(x, \sigma) = c(\lambda) e^{-\lambda S(x)} \rho(x, \sigma), \quad (1.1)$$

where $c(\lambda)$ is a normalization factor depending only on λ . Given the stationary measure ρ_λ , we consider the time–reversed (adjoint) version of the PDMP and we show that it is again a PDMP, with inverted vector fields and transition rates λr^+ which depend on the direct rates r and on the stationary measure ρ_λ . In particular, our PDMPs typically describe out–of–equilibrium systems, since reversibility appears only in the trivial case of vanishing force fields. For exactly solvable models as in (1.1), we can show that $r^+(\cdot, \cdot|x)$ does not depend on λ as well some symmetry relations.

In order to study the deviations of the system from its relaxation to equilibrium, we introduce a scaling procedure forcing the system to behave deterministically in the asymptotic limit. Simply, we take the limit $\lambda \uparrow \infty$. As result, the timescale of chemical jumps becomes infinitesimal w.r.t. the timescale of the mechanical evolution and the dynamics is a combination of slow and fast motions. As one would expect, an *averaging principle* holds: the slow motion is well approximated by averaging the effect of the fast motion, considering the fast (chemical) variable as locally equilibrated. In order to be more precise, let us assume that for any $x \in \Omega$ the continuous–time Markov chain on Γ with jump rates $r(\cdot, \cdot|x)$ (x being interpreted as frozen variable) is irreducible and therefore has a unique invariant probability measure $\mu(\cdot|x)$ on Γ . Then the above high frequency limit implies that, whenever the mechanical state of the PDMP is x , the chemical state is given by σ with probability well approximated by $\mu(\sigma|x)$, while with probability tending to 1 the mechanical evolution $x(t)$ is well approximated by the deterministic path $x_*(\cdot)$ solving the Cauchy system

$$\begin{cases} \dot{x}_*(t) = \bar{F}(x_*(t)), \\ x_*(0) = x_0, \end{cases} \quad (1.2)$$

x_0 being the initial mechanical state and \bar{F} being the averaged vector field

$$\bar{F}(x) = \sum_{\sigma \in \Gamma} \mu(\sigma|x) F_\sigma(x).$$

The above averaging principle corresponds to a law of large numbers for the mechanical evolution and, introducing suitable spaces and topologies, it can be extended to the joint evolution $(x(t), \sigma(t))$ (see Section 6). A rigorous derivation of the averaging principle as well as the large deviations (LD) principle for PDMPs can be found in the companion paper [12].

Considering the chemical variable as hidden and taking the limit $\lambda \uparrow \infty$, we analyze the structure of fluctuations of the mechanical variable, i.e. deviations from its asymptotic deterministic behavior (1.2), following ideas and results of [1, 2, 3, 4], for stochastic interacting particle systems. A key identity observed in [2] is the Fluctuation–Dissipation (FD) relation

$$\mathcal{L}(x, \dot{x}) = \nabla V(x) \cdot \dot{x} + \mathcal{L}^+(x, -\dot{x}), \quad (1.3)$$

where V denotes the static LD functional of the steady state (in exactly solvable models as in (1.1), $V = S$), while \mathcal{L} and \mathcal{L}^+ are such that the LD functionals for the dynamics of the PDMP and its time-reversed version are obtained by integrating along the mechanical trajectories $x(t)$ the functions $\mathcal{L}(x, \dot{x})$ and $\mathcal{L}^+(x, \dot{x})$, respectively. As observed in [1, 2, 3, 4] and recalled in Section 7, whenever the FD relation is satisfied, several physical properties concerning the relaxation of the system hold. In [2] the authors derive the above FD relation from the definition of the time-reversed process and from the Markov property of the processes under considerations (the direct one and the time-reversed one). In our case, the mechanical evolution $x(t)$ is typically non Markovian, hence the validity of the FD relation has to be investigated. When the dependence on the parameter λ of the transition rates λr^+ is linear or almost linear, as in the case of 1D system or in the case of exactly solvable model with stationary measure (1.1), we can apply again our LD principle for λ -rescaled PDMPs. Then, we show the validity of the FD relation for the entire class of solvable PDMPs whose stationary measures satisfies (1.1) as well for PDMPs with two chemical states on the one dimensional torus for which the stationary measure is not of the form (1.1).

We briefly discuss a Gallavotti–Cohen–type symmetry relation for PDMPs. The natural symmetry for this class of processes is different from time-reversal and the corresponding action functional has a direct physical interpretation. We obtain in this way examples answering a question raised at the end of Subsection (2.2) in [17]. See also [18] and [16] for more details and references on the Gallavotti–Cohen symmetry in the framework of stochastic dynamics.

The paper is structured as follows. In Section 2 we give a detailed description of the model and comment our basic assumptions. In Section 3 we discuss stationarity and reversibility, giving a system of differential equations with boundary conditions characterizing the stationary measure and showing that the adjoint process is again a PDMP. In Section 4 we compute the stationary measure for a class of 1D PDMPs, which in many cases has the special form (1.1). In Section 5 we outline a general method valid in all dimensions in order to determine stationary measures of the form (1.1), and we apply it in several examples. In Section 6 we recall the averaging and large deviation principles obtained in [12]. Having at this point all the necessary tools, in Section 7 we study the static and dynamical deviations of the system from its typical behavior in the same spirit of the fluctuation theory developed in [1, 2, 3, 4]. Finally, in Section 8 we study a Gallavotti–Cohen–type symmetry relation.

We conclude with a remark. Being stochastic dynamical systems, PDMPs can have very different behaviors and show special features. When possible we have tried to keep our analysis at a general level, thus requiring some mathematical abstraction. On the other hand, special dynamical mechanisms have been discussed directly by means of examples. Moreover, even in very simple examples standard stochastic tools used in the paper as the Markov generator can become very delicate and subtle. The interested reader can find some insights in the appendix and can refer to [10] for a general theory.

2. THE MODEL

We consider stochastic models with state space $\Omega \times \Gamma$, where Γ is a finite set and Ω is either a domain (i.e. open and connected subset) of \mathbb{R}^d with regular boundary $\partial\Omega$, or the closure of a domain of \mathbb{R}^d with regular boundary, or the d -dimensional torus $\mathbb{R}^d/\mathbb{Z}^d$. A generic element of the state space is denoted by (x, σ) . Inspired by power-stroke models

of molecular motors, we call the variables $x \in \Omega$ and $\sigma \in \Gamma$ the *mechanical state* and the *chemical state* of the system, respectively. Their joint stochastic evolution can be described as follows. The mechanical state x evolves continuously, while the chemical state σ jumps at random times. When the chemical state is σ , the mechanical state evolves according to the ordinary differential equation

$$\dot{x}(t) = F_\sigma(x(t)), \quad (2.1)$$

where, for any $\sigma \in \Gamma$, $F_\sigma(x) = (F_{\sigma,1}(x), \dots, F_{\sigma,d}(x)) \in \mathbb{R}^d$ is a vector field. If Ω is the d -dimensional torus, in the above equation x is thought of as element of a box in \mathbb{R}^d with periodic boundary conditions. We assume that the vector fields F_σ have continuous extension to the closure $\bar{\Omega}$ and satisfy the Lipschitz condition

$$|F_\sigma(x) - F_\sigma(y)| \leq K_\sigma |x - y|, \quad \forall x, y \in \Omega, \quad (2.2)$$

for appropriate constants K_σ . Moreover, we assume that the mechanical evolution remains confined inside the region Ω . This assumption together with (2.2) implies existence and uniqueness of the mechanical trajectory.

The chemical state σ performs a jump stochastic dynamics with rates depending on the mechanical state. More precisely, the jump rates are continuous functions $r(\sigma, \sigma'|x) : \Gamma \times \Gamma \times \Omega \rightarrow [0, \infty)$. Without loss of generality we assume that

$$r(\sigma, \sigma|x) = 0, \quad \forall (x, \sigma) \in \Omega \times \Gamma.$$

Moreover, we call $\gamma(\sigma|x) = \sum_{\sigma' \in \Gamma} r(\sigma, \sigma'|x)$. Given the initial state $(x_0, \sigma_0) \in \Omega \times \Gamma$, we consider the random variable τ_1 with distribution

$$\mathbb{P}(\tau_1 > t) = \begin{cases} e^{-\lambda \int_0^t \gamma(\sigma_0|x_0(s))ds} & t \geq 0, \\ 1 & t < 0. \end{cases}$$

In the above formula λ is a positive parameter and $x_0(s)$ is the solution of the Cauchy problem

$$\begin{cases} \dot{x}(t) = F_{\sigma_0}(x(t)), \\ x(0) = x_0. \end{cases} \quad (2.3)$$

The evolution of the system (mechanical state and chemical state) in the time interval $[0, \tau_1)$ is given by $(x_0(s), \sigma_0)$. The chemical state $\sigma(\tau_1)$ is then chosen in Γ according to the distribution

$$\mathbb{P}(\sigma(\tau_1) = \sigma) = \frac{r(\sigma_0, \sigma|x(\tau_1))}{\gamma(\sigma_0|x(\tau_1))}.$$

Let $x_1(t)$, $t \geq \tau_1$, be the solution of (2.3) for the vector field $F_{\sigma(\tau_1)}$ and initial condition $x_1(\tau_1) = x_0(\tau_1)$. Let τ_2 be a random variable distributed according to

$$\mathbb{P}(\tau_2 > t) = \begin{cases} e^{-\lambda \int_{\tau_1}^t \gamma(\sigma(\tau_1)|x_1(s))ds} & t \geq \tau_1, \\ 1 & t < \tau_1. \end{cases}$$

The evolution of the system in the time interval $[\tau_1, \tau_2)$ is given by $(x_1(s), \sigma(\tau_1))$. The chemical state $\sigma(\tau_2)$ is chosen in Γ according to the distribution

$$\mathbb{P}(\sigma(\tau_2) = \sigma) = \frac{r(\sigma(\tau_1), \sigma|x(\tau_2))}{\gamma(\sigma(\tau_1)|x(\tau_2))},$$

and so on. In general, we denote by τ_k the random time of the k -th chemical jump and by $(x_k(s), \sigma(\tau_k))$ the state of the system at time $s \in [\tau_k, \tau_{k+1})$. We have that $x_k(s)$ solves

(2.3) for the vector field $F_{\sigma(\tau_k)}$ with initial condition $x_k(\tau_k) := x_{k-1}(\tau_k)$ and that τ_{k+1} is a random variable with distribution

$$\mathbb{P}(\tau_{k+1} > t) = \begin{cases} e^{-\lambda \int_{\tau_k}^t \gamma(\sigma(\tau_k)|x_k(s))ds} & t \geq \tau_k, \\ 1 & t < \tau_k. \end{cases} \quad (2.4)$$

The chemical state $\sigma(\tau_{k+1})$ is then chosen in Γ according to the distribution

$$\mathbb{P}(\sigma(\tau_{k+1}) = \sigma) = \frac{r(\sigma(\tau_k), \sigma | x(\tau_{k+1}))}{\gamma(\sigma(\tau_k) | x(\tau_{k+1}))}.$$

In order to have a well-defined dynamics for all positive times we require that a.s. the family of jump times τ_k has no accumulation point. This is always true if $\lim_{k \uparrow \infty} \tau_k = +\infty$ a.s.

The natural path space of the process $(x(\cdot), \sigma(\cdot))$ is given by the cartesian product

$$C([0, T], \Omega) \times D([0, T], \Gamma). \quad (2.5)$$

The first component is the space of continuous functions from $[0, T]$ to Ω , while the second component is the Skorokhod space of functions from $[0, T]$ to Γ , which are right continuous and have left limits. We note that, due to relation (2.1), the mechanical trajectory $\{x(t)\}_{t \in [0, T]}$ is a piecewise differentiable function and it holds

$$\dot{x}(s) = F_{\sigma(s)}(x(s)), \quad (2.6)$$

for any $s \in [0, T]$ where $\{\sigma(t)\}_{t \in [0, T]}$ is continuous.

The above stochastic process $(x(\cdot), \sigma(\cdot))$ is called *Piecewise Deterministic Markov Process* (PDMP) [9], [10]. In control theory, it is a typical example of *stochastic hybrid system* [8]. Although the evolution of the mechanical state as well the evolution of the chemical state are not Markovian, as proven in [9], [10] the joint evolution $(x(\cdot), \sigma(\cdot))$ is a strong Markov process, whose Markov generator is formally

$$Lf(x, \sigma) = F_{\sigma}(x) \cdot \nabla f(x, \sigma) + \lambda \sum_{\sigma' \in \Gamma} r(\sigma, \sigma' | x) (f(x, \sigma') - f(x, \sigma)) \quad (2.7)$$

where $f : \Omega \times \Gamma \rightarrow \mathbb{R}$ is regular in the mechanical variable x . In Appendix A we will specify the precise meaning and domain of the operator L . For any fixed $x \in \Omega$, the x -dependent Markov generator $L_c[x]$ on Γ given by

$$L_c[x]f(\sigma) = \sum_{\sigma' \in \Gamma} r(\sigma, \sigma' | x) (f(\sigma') - f(\sigma)) \quad (2.8)$$

is called the *chemical part* of the generator L . Hence, we can write

$$Lf(x, \sigma) = F_{\sigma}(x) \cdot \nabla f(x, \sigma) + \lambda L_c[x]f(x, \sigma).$$

Note that $L_c[x]$ is the Markov generator of a continuous-time Markov chain on Γ where jumps from σ to σ' take place with probability rate $r(\sigma, \sigma' | x)$. We will assume that for any fixed $x \in \Omega$, this Markov chain is irreducible and consequently has a unique stationary measure $\mu(\cdot | x)$, that we call *quasistationary measure*. In the particular case of two chemical states, e.g. $\Gamma = \{0, 1\}$, this condition reduces to the positivity of the rates $r(0, 1 | x)$ and $r(1, 0 | x)$. In this case, the quasistationary measure is also reversible w.r.t. the Markov chain on Γ with generator $L_c[x]$ and is given by

$$\mu(0 | x) = \frac{r(1, 0 | x)}{r(0, 1 | x) + r(1, 0 | x)}, \quad \mu(1 | x) = \frac{r(0, 1 | x)}{r(0, 1 | x) + r(1, 0 | x)}. \quad (2.9)$$

Let us now come back to our assumptions and give some comments. As already stated, in order to have a well-defined dynamics for all positive times we require that a.s. the family of random jump times τ_k has no accumulation point. This fact is implied for example by the condition

$$\sup_{\{x \in \Omega\}} \max_{\{\sigma \in \Gamma\}} \gamma(\sigma|x) < \infty. \quad (2.10)$$

Indeed, calling C the l.h.s. of (2.10), due to (2.4) we get that $\mathbb{P}(\tau_{k+1} - \tau_k > t) \geq e^{-C\lambda t}$. This allows to build a coupling between the family of random jump times τ_k and a Poisson point process (PPP) on $(0, \infty)$ with density $C\lambda$ such that all jump times τ_k belong to the PPP. Since a.s. the PPP has no accumulation point, the same property holds for the family of jump times τ_k and this proves our claim. Let us also point out that, due to the above coupling, we get that the random variable N_t given by the number of jump times τ_k in the time interval $[0, t]$ has finite expectation.

One can even weaken condition (2.10). Due to the irreducibility assumption for $L_c[x]$, the absence of accumulation points for the family of jump times τ_k is implied by the condition

$$\sup_{\{x \in \Omega\}} \min_{\{\sigma \in \Gamma\}} \gamma(\sigma|x) < +\infty \quad (2.11)$$

and some other additional assumptions. Without trying to give some general criterion, in order to explain the mechanism we have in mind we discuss in Appendix B an example where (2.11) is valid and (2.10) is violated, while the family of jump times τ_k has no accumulation point.

As already stated, we assume that the mechanical trajectory $x(t)$ remains confined inside Ω . If Ω is the d -dimensional torus, this assumption is trivially satisfied. Let us consider the case $\Omega \subset \mathbb{R}^d$. Then, it is necessary that there is zero flux through the boundary. A sufficient condition is given by

$$F_\sigma(x) \cdot n(x) \leq 0, \quad \forall \sigma \in \Gamma, x \in \partial\Omega, \quad (2.12)$$

where \cdot denotes the Euclidean scalar product in \mathbb{R}^d , while $n(x)$ denotes the outward normal to $\partial\Omega$. If Ω includes its boundary $\partial\Omega$, the above condition is enough to have confinement, otherwise one can require in addition to (2.12) that

$$F_\sigma(x) = 0 \quad \forall x \in \partial\Omega \text{ s.t. } F_\sigma(x) \cdot n(x) = 0. \quad (2.13)$$

This condition excludes the presence of orbits tangent to the boundary at some point.

Another condition assuring the confinement of $x(t)$ is the following. We take $\Omega \subset \mathbb{R}^d$ open for simplicity. For any $\sigma \in \Gamma$ and $x_0 \in \partial\Omega$, consider the trajectory $x(t)$ starting in x_0 with reversed vector field $-F_\sigma(x)$, namely $\dot{x}(t) = -F_\sigma(x(t))$. If this trajectory is well defined in some time interval $[0, t_0)$ such that $x(t) \in \Omega$ for all $t \in (0, t_0)$, then we require that

$$\int_0^{t_0} \gamma(\sigma|x(s)) ds = +\infty. \quad (2.14)$$

We claim that the mechanical evolution is kept bounded inside Ω by a stochastic mechanism. In fact, condition (2.14) guarantees that if the mechanical trajectory is pointing towards x_0 , with probability one there is a jump to a new chemical state before reaching x_0 . Now again, if the mechanical trajectory associated to the new chemical state is pointing towards a point $x_1 \in \partial\Omega$, with probability one there is a jump to a new chemical state before reaching x_1 . In order to reach the boundary $\partial\Omega$ in a finite time, the system should perform infinite chemical jumps in that time interval, which is not possible due to our assumptions. In the examples discussed below, the above two criteria for the mechanical

confinement inside open Ω 's are dual: if the system is confined due to (2.12) and (2.13), the time-reversed system will be confined due to (2.14).

We will mainly be interested in models such that a.s. the family of random jumps times τ_k is infinite. A sufficient condition to obtain this behavior is given by

$$\inf_{\{x \in \Omega\}} \min_{\{\sigma \in \Gamma\}} \gamma(\sigma|x) > 0. \quad (2.15)$$

In fact, with arguments similar to the ones after (2.10), it can be shown that the family of jump times dominates a PPP. We discuss in Appendix C an example of a PDMP that violates (2.15) and has a.s. a finite number of chemical jumps.

Finally we remark that if there exists $x^* \in \Omega$ such that $F_\sigma(x^*) = 0$ for any $\sigma \in \Gamma$, then the PDMP with initial condition $x(0) = x^*$ has a trivial behavior: the mechanical variable does not evolve, while the chemical variable evolves as a continuous-time Markov chain with transition rates $r(\sigma, \sigma'|x^*)$.

We conclude this section with some notation frequently used below. Given a point $(x, \sigma) \in \Omega \times \Gamma$, we denote by $\mathbb{P}_{x, \sigma}^\lambda$ and $\mathbb{E}_{x, \sigma}^\lambda$ the law of the process $(x(\cdot), \sigma(\cdot))$ starting in (x, σ) and the associated expectation, respectively.

3. STATIONARITY AND REVERSIBILITY

A probability measure ρ_λ on $\Omega \times \Gamma$ is called *invariant*, or *stationary*, if for any time $t \geq 0$ the pair $(x(t), \sigma(t))$ is distributed according to ρ_λ when the process has initial distribution ρ_λ . In this case, the process starting with distribution ρ_λ is called stationary. Since the dynamics is defined by time-independent rules, this implies that for each $t \geq 0$ the laws of the trajectory $\{x(s), \sigma(s)\}_{s \geq 0}$ and the law of the time-shifted trajectory $\{x(s+t), \sigma(s+t)\}_{s \geq 0}$ coincide. This observation together with Kolmogorov Theorem allows to univocally extend the process for all times $t \in \mathbb{R}$, by requiring that its law does not change under time-shifts. Below, when referring to a stationary process we will often mean the \mathbb{R} -extended one. In particular, if the process is stationary we can define its time-reversed version. To this aim, we introduce the *time-reversal operator*, defined as

$$\mathcal{T}[\{x(t), \sigma(t)\}_{t \in \mathbb{R}}] := \{x(-t), \sigma(-t)\}_{t \in \mathbb{R}}. \quad (3.1)$$

Since we want \mathcal{T} to be an operator from and onto the path space $C(\mathbb{R}, \Omega) \times D(\mathbb{R}, \Gamma)$, the above definition has to be slightly modified by replacing the r.h.s. of (3.1) with the only path in $C(\mathbb{R}, \Omega) \times D(\mathbb{R}, \Gamma)$ coinciding with $\{x(-t), \sigma(-t)\}_{t \in \mathbb{R}}$ at all continuity points t . For the sake of simplicity, when writing the r.h.s. of (3.1) we will mean this last path. Then the *time-reversed process* (also called *adjoint process*) is defined as the process obtained from the original one via \mathcal{T} . If $\mathbb{P}_{\rho_\lambda}^\lambda$ is the law of the original process, then $\mathbb{P}_{\rho_\lambda}^{\lambda,+} := \mathbb{P}_{\rho_\lambda}^\lambda \circ \mathcal{T}^{-1}$ is the law of the time-reversed process. If the two laws coincide, one says that the process with law $\mathbb{P}_{\rho_\lambda}^\lambda$ is *reversible* and that ρ_λ is a reversible measure for the process. As we will explain below, the time-reversed process is again a PDMP. Due to the Markov property, by considering the transition probability kernels of $\mathbb{P}_{\rho_\lambda}^{\lambda,+}$, one can easily define the adjoint process with arbitrary initial distribution ν . We will denote $\mathbb{P}_\nu^{\lambda,+}$ its law on $C(\mathbb{R}_+, \Omega) \times D(\mathbb{R}_+, \Gamma)$.

Existence and uniqueness of the stationary measure of a PDMP can be non trivial and the analysis can be very model-dependent. If Ω is bounded one can deduce the existence of a stationary measure as follows. Fixed any initial distribution ν , we write ν_s for the law of

$(x(s), \sigma(s))$ under \mathbb{P}_ν^λ . By compactness arguments (cf. [6]), the family of Cesaro averages $\tilde{\nu}_t := t^{-1} \int_0^t \nu_s ds$ admits a subsequence $\tilde{\nu}_{t_n}$, with $t_n \uparrow \infty$, converging to some probability measure ν_* on $\bar{\Omega} \times \Gamma$. If Ω is closed or if Ω is open and $\nu_*(\partial\Omega) = 0$, then by standard arguments one can show that ν_* is a stationary probability measure for the PDMP. The fact that $\nu_*(\partial\Omega) = 0$ for $\Omega \subset \mathbb{R}^d$ can be verified for example if, when approaching the boundary, the system typically jumps to a chemical state σ with a vector field F_σ of order one pointing inside Ω . We will come back to this mechanism in Appendix B. Other existence criteria are given in [10].

In the rest of this section we restrict to the case of $\Omega \subset \mathbb{R}^d$ open or Ω being a d -dimensional torus. Assuming now the existence of some stationary measure ρ_λ , we want to give a characterization of ρ_λ by means of partial differential equations. Due to Theorem 34.19 in [10], if ρ_λ is a stationary measure then it must be

$$\rho_\lambda(Lf) = 0 \quad (3.2)$$

for a large class of functions f in the domain of the extended generator (see Appendix A for the definition of extended generator) and in particular for functions f which are bounded and C^1 in x . Let us denote here by \mathbb{F} the family of functions f which are C^1 in x , have continuous extension to $\partial\Omega$ and satisfy for some σ the property: $f(x, \sigma') = 0$ if $\sigma' \neq \sigma$. Assuming $\rho_\lambda = \sum_\sigma \rho_\lambda(x, \sigma) dx d\sigma$ (i.e. ρ_λ is absolutely continuous w.r.t. the Lebesgue measure on each subspace $\Omega \times \{\sigma\}$) and assuming that $\rho_\lambda(\cdot, \sigma)$ is C^1 , equation (3.2) for $f \in \mathbb{F}$ reads

$$\int_\Omega dx \rho_\lambda(x, \sigma) F_\sigma(x) \cdot \nabla f(x, \sigma) + \lambda \sum_{\sigma' \in \Gamma} \int_\Omega dx f(x, \sigma) (\rho_\lambda(x, \sigma') r(\sigma', \sigma) - \rho_\lambda(x, \sigma) r(\sigma, \sigma')) = 0. \quad (3.3)$$

By the Gauss–Green formula, the first integral in the l.h.s. equals

$$\int_{\partial\Omega} dS(x) f(x, \sigma) \rho_\lambda(x, \sigma) F_\sigma(x) \cdot n(x) - \int_\Omega dx f(x, \sigma) \nabla \cdot (\rho_\lambda(x, \sigma) F_\sigma(x)), \quad (3.4)$$

where dS denotes the $(d-1)$ -dimensional surface measure on $\partial\Omega$ and $n(x)$ denotes the outward normal to $\partial\Omega$ in x . Since (3.3) must hold in particular for all functions $f \in \mathbb{F}$ with x -support given by a compact subset of Ω , we conclude that

$$\lambda \sum_{\sigma' \in \Gamma} \left(\rho_\lambda(x, \sigma') r(\sigma', \sigma | x) - \rho_\lambda(x, \sigma) r(\sigma, \sigma' | x) \right) = \nabla \cdot (\rho_\lambda(x, \sigma) F_\sigma(x)), \quad \forall (x, \sigma) \in \Omega \times \Gamma. \quad (3.5)$$

Then, due to (3.3), (3.4) and (3.5), the boundary integral in (3.4) must be zero for all functions $f \in \mathbb{F}$. This forces ρ_λ to have zero flux across the boundary $\partial\Omega$:

$$\left(\rho_\lambda(x, \sigma) F_\sigma(x) \cdot n(x) \right) \Big|_{x \in \partial\Omega} = 0, \quad \forall \sigma \in \Gamma. \quad (3.6)$$

Note that if Ω is the closure of a domain in \mathbb{R}^d , the system of identities (3.5) must still be valid for $(x, \sigma) \in \Omega^\circ \times \Gamma$, Ω° being the interior part of Ω , since it follows from (3.2) by taking arbitrary functions f which are bounded, C^1 in x and with x -support strictly included in Ω° . The boundary condition can differ from (3.6), depending on the dynamics at the boundary.

As already mentioned, if the process $\mathbb{P}_{\rho_\lambda}^\lambda$ is stationary, then its time-reversed version is again a PDMP. More precisely, we claim that $\mathbb{P}_{\rho_\lambda}^{\lambda,+}$ coincides with the law P of the PDMP

with state space $\Omega \times \Gamma$, initial distribution ρ_λ , force fields

$$F_\sigma^+(x) := -F_\sigma(x) \quad (3.7)$$

and jump rates $\lambda r^+(\sigma, \sigma'|x)$ where

$$r^+(\sigma, \sigma'|x) := r(\sigma', \sigma|x) \frac{\rho_\lambda(x, \sigma')}{\rho_\lambda(x, \sigma)}. \quad (3.8)$$

(In the above formula, we assume some spatial irreducibility of the system implying the positivity of $\rho_\lambda(x, \sigma)$). Note that writing

$$\gamma^+(\sigma|x) := \sum_{\sigma'} r^+(\sigma, \sigma'|x), \quad (3.9)$$

equation (3.5) can be written as

$$\lambda(\gamma^+(\sigma|x) - \gamma(\sigma|x)) = \frac{\nabla \cdot (\rho_\lambda(x, \sigma) F_\sigma(x))}{\rho_\lambda(x, \sigma)}. \quad (3.10)$$

In order to prove our claim, due to the stationarity of $\mathbb{P}_{\rho_\lambda}^\lambda$ we only need to show that

$$P(A) = \mathbb{P}_{\rho_\lambda}^\lambda(B), \quad (3.11)$$

where the events A and B are of the following form. Fix a measurable set $U \subset \Omega$, $k+1$ chemical states $\sigma_0, \sigma_1, \dots, \sigma_k$ with $\sigma_i \neq \sigma_{i+1}$, k positive times $0 < t_1 < \dots < t_k < T$ and ϵ small enough. Define A as the family of paths $(x(\cdot), \sigma(\cdot)) \in C(\mathbb{R}_+, \Omega) \times D(\mathbb{R}_+, \Gamma)$ such that (i) there are exactly k jump times $\tau_1, \tau_2, \dots, \tau_k$ in the time interval $(0, T)$ and $\tau_i \in [t_i - \epsilon, t_i + \epsilon]$, (ii) $\sigma(\tau_i) = \sigma_i$ for $0 < i \leq k$ and moreover $\sigma(0) = \sigma_0$, (iii) $x(0) \in U$ and (iv) $\dot{x}(s) = -F_{\sigma(s)}(x(s))$ for all $s \in [0, T)$ different from the jump times. Then define B as the family of paths $(x(\cdot), \sigma(\cdot))$ such that (i) there are exactly k jumps times τ'_1, \dots, τ'_k in the time interval $[0, T]$ and $\tau'_i \in [T - t_{k-i+1} - \epsilon, T - t_{k-i+1} + \epsilon]$, (ii) $\sigma(\tau'_i) = \sigma_{k-i}$ for $1 \leq i \leq k$ and moreover $\sigma(0) = \sigma_k$, (iii) $x(T) \in U$ and (iv) $\dot{x}(s) = F_{\sigma(s)}(x(s))$ for all $s \in [0, T]$ different from the jump times. Trivially, apart time-shift A and $\mathcal{T}^{-1}B$ coincide. Note that the validity of (3.11) for all events A and B as above implies also that P gives probability 1 to paths with mechanical variable confined in Ω .

For the sake of simplicity and without loss of generality, in order to prove (3.11) we take $k = 1$. Moreover, given $x_0 \in U$ and $t \in [t_1 - \epsilon, t_1 + \epsilon]$, we write $(x(\cdot), \sigma(\cdot))$ for the unique path in A jumping at time t and such that $x(0) = x_0$. Then, due to (3.8), (3.9) and (3.10), we conclude that

$$P(A) = \int_{t_1 - \epsilon}^{t_1 + \epsilon} g_t dt, \quad (3.12)$$

where the density g_t is given by

$$\begin{aligned} g_t &= \lambda \int_U dx_0 \rho_\lambda(x_0, \sigma_0) r^+(\sigma_0, \sigma_1|x(t)) \exp\left\{-\lambda \int_0^T \gamma^+(\sigma(s)|x(s)) ds\right\} \\ &= \lambda \int_U dx_0 \rho_\lambda(x_0, \sigma_0) \frac{\rho_\lambda(x(t), \sigma_1)}{\rho_\lambda(x(t), \sigma_0)} r(\sigma_1, \sigma_0|x(t)) \\ &\quad \times \exp\left\{-\lambda \int_0^T \gamma(\sigma(s)|x(s)) ds\right\} \exp\left\{-\int_0^T \frac{\nabla \cdot (\rho_\lambda(x(s), \sigma(s)) F_{\sigma(s)}(x(s)))}{\rho_\lambda(x(s), \sigma(s))} ds\right\}. \end{aligned} \quad (3.13)$$

We note that in the time intervals $(0, t)$ and (t, T) where the chemical state is constant, it holds

$$\frac{\nabla \cdot (\rho_\lambda(x(s), \sigma) F_\sigma(x(s)))}{\rho_\lambda(x(s), \sigma)} = -\frac{d}{ds} \ln \rho_\lambda(x(s), \sigma) + \nabla \cdot F_\sigma(x(s)),$$

where σ is the value of the chemical state. Dividing the interval of integration $[0, T]$ in the two intervals $[0, t]$ and $[t, T]$, the above identity implies that the last exponential factor in (3.13) equals

$$\frac{\rho_\lambda(x(t), \sigma_0) \rho_\lambda(x(T), \sigma_1)}{\rho_\lambda(x_0, \sigma_0) \rho_\lambda(x(t), \sigma_1)} \exp \left\{ - \int_0^T \nabla \cdot F_{\sigma(s)}(x(s)) ds \right\}.$$

This observation together with (3.13) allows to conclude that

$$g_t = \lambda \int_U dx_0 \rho_\lambda(x(T), \sigma_1) r(\sigma_1, \sigma_0 | x(t)) \times \exp \left\{ -\lambda \int_0^T \gamma(\sigma(s) | x(s)) ds \right\} \exp \left\{ - \int_0^T \nabla \cdot F_{\sigma(s)}(x(s)) ds \right\}. \quad (3.14)$$

Let us now consider the diffeomorphism $\phi : U \rightarrow \phi(U)$ that associate to $x_0 \in U$ the element $x(T) \in \phi(U)$. This is obtained from the composition $\phi_2 \circ \phi_1$ where ϕ_1 maps x_0 to $x(t)$ and ϕ_2 maps $x(t)$ to $x(T)$. By Liouville theorem the Jacobian J_{ϕ_1} of the diffeomorphism ϕ_1 is given by

$$J_{\phi_1}(x_0) = e^{-\int_0^t \nabla \cdot F_{\sigma_0}(x(s)) ds}, \quad (3.15)$$

and the Jacobian J_{ϕ_2} of the diffeomorphism ϕ_2 is given by

$$J_{\phi_1}(x(t)) = e^{-\int_t^T \nabla \cdot F_{\sigma_1}(x(s)) ds}. \quad (3.16)$$

If we perform in (3.14) the change of variables $y_0 = \phi(x_0)$ we obtain

$$g_t = \lambda \int_{\phi(U)} dy_0 \rho_\lambda(y_0, \sigma_1) r(\sigma_1, \sigma_0 | y(T-t)) \exp \left\{ -\lambda \int_0^T \gamma(\sigma(s) | y(s)) ds \right\} := \tilde{g}_{T-t}, \quad (3.17)$$

where $(y(\cdot), \sigma(\cdot))$ is the unique path in B jumping at time $T-t$ and such that $y(0) = y_0$. Now (3.11) follows from (3.12) and the identity

$$\mathbb{P}_{\rho_\lambda}^\lambda(B) = \int_{T-t_1-\epsilon}^{T-t_1+\epsilon} \tilde{g}_t dt.$$

A different route in order to characterize the time-reversed process is given by the analysis of the generator. Being aware of the subtle difficulties concerning the domain of definition of the generator (see Appendix A), we keep this analysis at a very heuristic level. The generator L^+ of the time-reversed process must be the adjoint in $L^2(\rho_\lambda)$ of the generator L of the direct process, namely

$$\mathbb{E}_{\rho_\lambda}(gLf) = \mathbb{E}_{\rho_\lambda}(fL^+g) \quad (3.18)$$

for all f, g regular enough. Below we check that this implies the identity

$$L^+f(x, \sigma) = -F_\sigma(x) \cdot \nabla f(x, \sigma) + \lambda \sum_{\sigma' \in \Gamma} r(\sigma', \sigma | x) \frac{\rho_\lambda(x, \sigma')}{\rho_\lambda(x, \sigma)} (f(x, \sigma') - f(x, \sigma)). \quad (3.19)$$

We can write (3.19) as

$$L^+f(x, \sigma) = -F_\sigma(x) \cdot \nabla f(x, \sigma) + \lambda L_c^+[x]f(x, \sigma). \quad (3.20)$$

We stress that $L_c^+[x]$ denotes the chemical part of the adjoint generator L^+ . In general, this is different from the operator $L_c[x]^+$, defined as the adjoint in $L^2(\mu(\cdot|x))$ of the chemical part $L_c[x]$ of the generator L :

$$L_c^+[x] \neq L_c[x]^+. \quad (3.21)$$

The general formula (3.19) can be easily checked as follows. We start from the left hand side of (3.18) that can be written as

$$\sum_{\sigma \in \Gamma} \int_{\Omega} dx \rho_{\lambda}(x, \sigma) g(x, \sigma) \left[F_{\sigma}(x) \cdot \nabla f(x, \sigma) + \lambda \sum_{\sigma' \in \Gamma} r(\sigma, \sigma'|x) (f(x, \sigma') - f(x, \sigma)) \right].$$

With a change of variable in the discrete sum and an integration by parts in the mechanical variable for which the boundary terms disappear due to conditions (3.6), we obtain

$$\begin{aligned} \sum_{\sigma \in \Gamma} \int_{\Omega} dx f(x, \sigma) \left\{ -\nabla \cdot \left(\rho_{\lambda}(x, \sigma) g(x, \sigma) F_{\sigma}(x) \right) \right. \\ \left. + \lambda \sum_{\sigma' \in \Gamma} \left(r(\sigma', \sigma|x) \rho_{\lambda}(x, \sigma') g(x, \sigma') - r(\sigma, \sigma'|x) \rho_{\lambda}(x, \sigma) g(x, \sigma) \right) \right\}. \end{aligned}$$

Using now (3.5) we get

$$\begin{aligned} \sum_{\sigma \in \Gamma} \int_{\Omega} dx f(x, \sigma) \left\{ -\nabla \cdot \left(\rho_{\lambda}(x, \sigma) g(x, \sigma) F_{\sigma}(x) \right) + g(x, \sigma) \nabla \cdot \left(\rho_{\lambda}(x, \sigma) F_{\sigma}(x) \right) \right. \\ \left. + \rho_{\lambda}(x, \sigma) \lambda \sum_{\sigma' \in \Gamma} \left(r(\sigma', \sigma|x) \frac{\rho_{\lambda}(x, \sigma')}{\rho_{\lambda}(x, \sigma)} g(x, \sigma') - r(\sigma, \sigma'|x) \frac{\rho_{\lambda}(x, \sigma')}{\rho_{\lambda}(x, \sigma)} g(x, \sigma) \right) \right\}, \end{aligned}$$

that finally becomes

$$\sum_{\sigma \in \Gamma} \int_{\Omega} dx \rho_{\lambda}(x, \sigma) f(x, \sigma) \left[-F_{\sigma}(x) \cdot \nabla g(x, \sigma) + \lambda \sum_{\sigma' \in \Gamma} r(\sigma', \sigma|x) \frac{\rho_{\lambda}(x, \sigma')}{\rho_{\lambda}(x, \sigma)} (g(x, \sigma') - g(x, \sigma)) \right].$$

This ends the proof of (3.19).

Let us conclude this section with some comments. We have showed that the time-reversed process is still a PDMP with reversed vector fields and with probability rates of chemical transitions given by (3.8). Note that in general these rates can be λ -dependent, thus implying that the chemical part of the adjoint generator can also be λ -dependent. Moreover, the chemical part of the adjoint generator $L_c^+[x]$ is irreducible for all $x \in \Omega$, due to the irreducibility of $L_c[x]$ and the identity (3.8). We call $\mu^+(\cdot|x)$ the quasistationary measure associated to $L_c^+[x]$ and we remark that it can be λ dependent. As already observed $L_c^+[x]$ and $L_c[x]$ are not adjoint operators w.r.t. quasistationary measure $\mu(\cdot|x)$. Another consequence of our results is the following: if for any fixed $x \in \Omega$ the chemical part $L_c[x]$ of the direct generator L is reversible with respect to the quasistationary measure $\mu(\cdot|x)$, then also the chemical part of the adjoint process $L_c^+[x]$ is reversible with respect to its quasistationary measure $\mu^+(\sigma|x)$ and moreover it holds

$$\mu^+(\sigma|x) = \frac{\rho_{\lambda}^2(x, \sigma)}{\mu(\sigma|x) Z_{\lambda}(x)}, \quad (3.22)$$

where $Z_{\lambda}(x)$ is the normalization constant. In order to justify (3.22), one can argue as follows. The reversibility of $L_c[x]$ is equivalent to the detailed balance condition

$$\mu(\sigma|x) r(\sigma, \sigma'|x) = \mu(\sigma'|x) r(\sigma', \sigma|x), \quad \forall \sigma, \sigma', \forall x \in \Omega. \quad (3.23)$$

Due to (3.8), this relation is equivalent to

$$\mu(\sigma|x)r^+(\sigma', \sigma|x) \frac{\rho_\lambda(x, \sigma')}{\rho_\lambda(x, \sigma)} = \mu(\sigma'|x)r^+(\sigma, \sigma'|x) \frac{\rho_\lambda(x, \sigma)}{\rho_\lambda(x, \sigma')},$$

that can be written as

$$\frac{\rho_\lambda^2(x, \sigma')}{\mu(\sigma'|x)} r^+(\sigma', \sigma|x) = \frac{\rho_\lambda^2(x, \sigma)}{\mu(\sigma|x)} r^+(\sigma, \sigma'|x).$$

This equation states that the rates r^+ at x satisfy the detailed balance condition with respect to a measure on Γ proportional to $\frac{\rho_\lambda^2(x, \sigma)}{\mu(\sigma|x)}$. The proportionality factor can depend on x and on λ . This is exactly the content of equation (3.22).

Finally, a comment about reversibility: due to our results, the direct PDMP can be reversible only if all the vector fields F_σ are identically zero. In this case the mechanical state remains constant and the model reduces to the continuous time Markov chain $\sigma(\cdot)$.

4. ONE DIMENSIONAL MODELS WITH TWO CHEMICAL STATES

In this section we discuss in detail some 1D models with two chemical states, for which it is possible to compute explicitly the invariant measure. We consider separately the cases of Ω interval and 1D torus. For simplicity we consider vector fields without equilibrium points in Ω , although the main ideas presented here can be used in more general cases.

4.1. Interval. We take $\Omega = (a, b) \subset \mathbb{R}$ and $\Gamma = \{0, 1\}$. In order to have some mixing and confinement inside Ω , we consider vector fields F_0, F_1 such that (i) $F_0(x) < 0$ and $F_1(x) > 0$ for all $x \in (a, b)$, (ii) $F_0(a) = F_1(b) = 0$. Because of the irreducibility of the Markov chain associated to $L_c[x]$, the jump rates $r(0, 1|x)$ and $r(1, 0|x)$ must be positive for all $x \in (a, b)$. The stationarity equations (3.5) are given by

$$\begin{cases} \lambda(\rho_\lambda(x, 1)r(1, 0|x) - \rho_\lambda(x, 0)r(0, 1|x)) &= \partial_x(\rho_\lambda(x, 0)F_0(x)), \\ \lambda(\rho_\lambda(x, 0)r(0, 1|x) - \rho_\lambda(x, 1)r(1, 0|x)) &= \partial_x(\rho_\lambda(x, 1)F_1(x)), \end{cases} \quad (4.1)$$

from which we obtain

$$\partial_x(\rho_\lambda(x, 0)F_0(x) + \rho_\lambda(x, 1)F_1(x)) = 0,$$

and consequently

$$\rho_\lambda(x, 0)F_0(x) + \rho_\lambda(x, 1)F_1(x) = c. \quad (4.2)$$

Due to the boundary condition (3.6), we know that c must be zero. Then relation (4.2) allows to solve equations (4.1) by separation of variables, leading to

$$\rho_\lambda(x, i) = \frac{e^{-\lambda \int_{x_*}^x \left(\frac{r(0, 1|z)}{F_0(z)} + \frac{r(1, 0|z)}{F_1(z)} \right) dz}}{Z|F_i(x)|}, \quad i = 0, 1, \quad (4.3)$$

where x_* is a generic element of (a, b) and Z is the normalization constant, if it exists. Note that the boundary condition (3.6) is automatically satisfied, since by construction the constant c in (4.2) is zero and by assumption $F_0(a) = F_1(b) = 0$. As the reader can check, (4.3) is the only solution of (3.5) compatible with the boundary condition (3.6). It corresponds to a probability measure if and only if the normalization constant Z is well-defined. Suppose for example that the jump rates vary in the interval (c_1, c_2) with $c_1, c_2 > 0$, while $F_1(x)$ and $F_0(x)$ are of order one near a and b respectively. Then it is simple to check that Z is well defined.

Knowing the stationary measure ρ_λ , we can compute via (3.8) the jump rates of the time-reversed process:

$$\begin{cases} r^+(0, 1|x) = r(1, 0|x) \frac{|F_0(x)|}{|F_1(x)|}, \\ r^+(1, 0|x) = r(0, 1|x) \frac{|F_1(x)|}{|F_0(x)|}. \end{cases}$$

We point out that these rates do not depend on λ . Moreover, we observe that in the reversed-time process the Ω -confinement is related to (2.14), while in the direct process the Ω -confinement is related by (2.12).

4.2. Torus. We take $\Omega = \mathbb{R}/\mathbb{Z}$, $\Gamma = \{0, 1\}$ and periodic vector fields $F_0(x)$, $F_1(x)$. We assume $F_0(x)$ and $F_1(x)$ to be nonzero. Moreover, in order to assure the irreducibility of the Markov chain associated to $L_c[x]$, we take positive jump rates $r(0, 1|x)$ and $r(1, 0|x)$. The equations for the stationary measure are still (4.1) to which we have to add the periodic boundary conditions

$$\rho_\lambda(0, i) = \rho_\lambda(1, i), \quad i = 0, 1. \quad (4.4)$$

Let us call

$$S(x) := \int_0^x \left(\frac{r(0, 1|z)}{F_0(z)} + \frac{r(1, 0|z)}{F_1(z)} \right) dz, \quad x \in \mathbb{R}. \quad (4.5)$$

It is easy to check that, for any constant k ,

$$\begin{cases} \rho_\lambda(x, 0) := \frac{k}{F_0(x)} \int_x^{x+1} \left[\frac{r(1, 0|y)}{F_1(y)} e^{\lambda(S(y)-S(x))} \right] dy, \\ \rho_\lambda(x, 1) := \frac{k}{F_1(x)} \int_x^{x+1} \left[\frac{r(0, 1|y)}{F_0(y)} e^{\lambda(S(y)-S(x))} \right] dy, \end{cases} \quad (4.6)$$

are solutions of (4.1), satisfying the boundary conditions (4.4), since for any $x, y \in \mathbb{R}$ it holds

$$S(y) - S(x) = S(y+1) - S(x+1). \quad (4.7)$$

Moreover, there exists a unique value of k such that the expressions in the r.h.s. of (4.6) are positive functions, satisfying the normalization condition

$$\sum_{\sigma=0,1} \int_0^1 \rho_\lambda(x, \sigma) dx = 1.$$

On the other hand, it is simple to check that the above solution is the only probability measure satisfying (3.5) and the periodic boundary conditions. Hence, we have obtained the unique invariant measure of the model.

Knowing the stationary measure ρ_λ , we can compute the jump rates of the time-reversed process:

$$\begin{cases} r^+(0, 1|x) = r(1, 0|x) \frac{F_0(x)}{F_1(x)} \frac{\int_x^{x+1} \left[\frac{r(0, 1|y)}{F_0(y)} e^{\lambda S(y)} \right] dy}{\int_x^{x+1} \left[\frac{r(1, 0|y)}{F_1(y)} e^{\lambda S(y)} \right] dy}, \\ r^+(1, 0|x) = r(0, 1|x) \frac{F_1(x)}{F_0(x)} \frac{\int_x^{x+1} \left[\frac{r(1, 0|y)}{F_1(y)} e^{\lambda S(y)} \right] dy}{\int_x^{x+1} \left[\frac{r(0, 1|y)}{F_0(y)} e^{\lambda S(y)} \right] dy}. \end{cases} \quad (4.8)$$

Note that in general, the above rates are λ -dependent. In order to exhibit cases of λ -independent rates $r^+(\cdot, \cdot|x)$, let us consider the *equilibrium condition*

$$\int_0^1 \left(\frac{r(0, 1|z)}{F_0(z)} + \frac{r(1, 0|z)}{F_1(z)} \right) dz = 0. \quad (4.9)$$

We point out that this condition can hold only if the vector fields F_0 and F_1 have opposite sign and that it is equivalent to the fact that S is a periodic function of period one. We

claim that the rates $r^+(\cdot, \cdot|x)$ do not depend on λ if the above equilibrium condition is satisfied. In fact, in this case, from the definition of S and from its periodicity we obtain that

$$\int_x^{x+1} \left[\left(\frac{r(1, 0|y)}{F_1(y)} + \frac{r(0, 1|y)}{F_0(y)} \right) e^{\lambda S(y)} \right] dy = \frac{1}{\lambda} \left(e^{\lambda S(x+1)} - e^{\lambda S(x)} \right) = 0. \quad (4.10)$$

From (4.8) and (4.10) we conclude that

$$\begin{cases} r^+(0, 1|x) = -r(1, 0|x) \frac{F_0(x)}{F_1(x)}, \\ r^+(1, 0|x) = -r(0, 1|x) \frac{F_1(x)}{F_0(x)}. \end{cases} \quad (4.11)$$

Remember that in this case the vector fields have opposite sign so that the above rates are positive.

When condition (4.9) is violated then rates (4.8) can be λ -dependent. In this case we can study the asymptotic behavior of ρ_λ as $\lambda \uparrow \infty$ using some classical results (see for example [7]) that we recall for the reader's convenience. Let f and S be smooth real functions on the interval $[a, b]$. If $S(y) < S(a)$ for any $y \in (a, b]$ and $S'(a) < 0$, then it holds

$$\lim_{\lambda \rightarrow \infty} \frac{\int_a^b f(y) e^{\lambda S(y)} dy}{e^{\lambda S(a)} \lambda^{-1}} = -\frac{f(a)}{S'(a)}. \quad (4.12)$$

If there exists $y^* \in (a, b)$ such that $S(y) < S(y^*)$ for any $y \in (a, b)$ different from y^* and moreover $S''(y^*) < 0$, then it holds

$$\lim_{\lambda \rightarrow \infty} \frac{\int_a^b f(y) e^{\lambda S(y)} dy}{e^{\lambda S(y^*)} \lambda^{-\frac{1}{2}}} = f(y^*) \sqrt{-\frac{2\pi}{S''(y^*)}}. \quad (4.13)$$

Let us suppose that the function S defined by (4.5) is regular and that for any $x \geq 0$ the maximum of the function S in the closed interval $[x, x+1]$ is assumed in at most one point of the open interval $(x, x+1)$. This fact is guaranteed if for example $S(z_1) \neq S(z_2)$ for any pair of critical points z_1 and z_2 (i.e. such that $S'(z_1) = S'(z_2) = 0$). If F_0 and F_1 have the same sign, this is always true since the function S is strictly increasing or strictly decreasing. Moreover, note that in general x and $x+1$ cannot be both maximum points of the function S on $[x, x+1]$, since due to (4.7) the identity $S(x) = S(x+1)$ would imply the periodicity of S . In addition to the previous assumptions, we require that $S''(y) < 0$ if the maximum of S on the interval $[x, x+1]$ is reached at the internal point y . We point out that by the methods discussed in [7] more general cases can be considered.

Given $x \geq 0$, we define $y(x) \in [x, x+1]$ as follows. We require that $S(y(x)) = \max_{y \in [x, x+1]} S(y)$. If the maximum point in $[x, x+1]$ is unique, then $y(x)$ is univocally determined from the above condition. The only other possibility is that there is a maximum point at the boundary and a maximum point in the interior of the interval $[x, x+1]$. In this case, we define $y(x)$ as the unique maximum point inside $(x, x+1)$.

From the results (4.12) and (4.13) it is easy to derive that

$$\begin{cases} r^+(0, 1|x) = r(1, 0|x) \frac{F_0(x)}{F_1(x)} \frac{r(0, 1|y(x)) F_1(y(x))}{r(1, 0|y(x)) F_0(y(x))} + o(1), \\ r^+(1, 0|x) = r(0, 1|x) \frac{F_1(x)}{F_0(x)} \frac{r(1, 0|y(x)) F_0(y(x))}{r(0, 1|y(x)) F_1(y(x))} + o(1), \end{cases} \quad (4.14)$$

where by $o(1)$ we indicate a term which is infinitesimal as λ diverges. Note that the first terms in the r.h.s. of (4.14) are λ -independent.

Note that if $y(x) \in \{x, x+1\}$, by the periodicity of $F_\sigma(x)$ and $r(\sigma, \sigma'|x)$ formula (4.14) reduces to

$$\begin{cases} r^+(0, 1|x) = r(0, 1|x) + o(1), \\ r^+(1, 0|x) = r(1, 0|x) + o(1). \end{cases} \quad (4.15)$$

This is always true if the vector fields F_0 and F_1 have the same sign, since in this case the function S is monotone. On the other hand, if $y(x) \in (x, x+1)$, then necessarily it holds

$$S'(y(x)) = \frac{r(0, 1|y(x))}{F_0(y(x))} + \frac{r(1, 0|y(x))}{F_1(y(x))} = 0, \quad (4.16)$$

and (4.14) reduces to

$$\begin{cases} r^+(0, 1|x) = -r(1, 0|x) \frac{F_0(x)}{F_1(x)} + o(1), \\ r^+(1, 0|x) = -r(0, 1|x) \frac{F_1(x)}{F_0(x)} + o(1). \end{cases} \quad (4.17)$$

We conclude this section by pointing out another consequence of the equilibrium condition (4.9), which we know to be equivalent to the periodicity of the function S . Setting

$$C(\lambda) = \int_0^1 \left[\frac{r(1, 0|y)}{F_1(y)} e^{\lambda S(y)} \right] dy,$$

due to (4.10), equations (4.6) read

$$\begin{cases} \rho_\lambda(x, 0) := \frac{kC(\lambda)}{F_0(x)} e^{-\lambda S(x)}, \\ \rho_\lambda(x, 1) := \frac{-kC(\lambda)}{F_1(x)} e^{-\lambda S(x)}. \end{cases} \quad (4.18)$$

5. EXACTLY SOLVABLE MODELS

In general it is difficult to obtain a closed expression for the invariant measure of our PDMPs. In this section we discuss a class of models for which this is possible and the invariant measure has a special structure.

5.1. General framework. The exact solutions of the 1D models discussed in the previous section suggest to look for invariant measures of the form

$$\rho_\lambda(x, \sigma) = c(\lambda) e^{-\lambda S(x)} \rho(x, \sigma), \quad (5.1)$$

where $c(\lambda)$ is a normalization factor depending only on λ , $S(x)$ is a function depending only on x and $\rho(x, \sigma)$ is a measure density on $\Omega \times \Gamma$ non depending on λ .

Let us discuss some consequences of (5.1) (other aspects will be discussed later, when studying the fluctuations of our models). If the PDMP has invariant measure of the form (5.1), then the rates r^+ of the adjoint process do not depend on λ :

$$r^+(\sigma, \sigma'|x) = r(\sigma', \sigma|x) \frac{\rho(x, \sigma')}{\rho(x, \sigma)}. \quad (5.2)$$

In particular, the chemical part $L_c^+[x]$ of the adjoint generator L^+ does not depend on λ . This implies that the quasistationary measure $\mu^+(\cdot|x)$ does not depend on λ . Moreover, if $L_c[x]$ is reversible with respect to the quasistationary measure $\mu(\cdot|x)$, then (3.22) becomes

$$\mu^+(\sigma|x) = \frac{\rho^2(x, \sigma)}{\mu(\sigma|x)Z(x)}. \quad (5.3)$$

Let us analyze now when (5.1) can be a solution of the stationary equations (3.5). Examples will be discussed at the end of this section. Inserting (5.1) in (3.5), we obtain that for any $\sigma \in \Gamma$ it must hold

$$\begin{aligned} \lambda c(\lambda) e^{-\lambda S(x)} \sum_{\sigma' \in \Gamma} \left(\rho(x, \sigma') r(\sigma', \sigma | x) - \rho(x, \sigma) r(\sigma, \sigma' | x) \right) = \\ -\lambda c(\lambda) e^{-\lambda S(x)} \nabla S(x) \cdot \left(\rho(x, \sigma) F_\sigma(x) \right) + c(\lambda) e^{-\lambda S(x)} \nabla \cdot \left(\rho(x, \sigma) F_\sigma(x) \right). \end{aligned} \quad (5.4)$$

Dividing by nonzero terms we get

$$\lambda \left[\sum_{\sigma' \in \Gamma} \left(\rho(x, \sigma') r(\sigma', \sigma | x) - \rho(x, \sigma) r(\sigma, \sigma' | x) \right) + \nabla S(x) \cdot \left(\rho(x, \sigma) F_\sigma(x) \right) \right] \quad (5.5)$$

$$+ \nabla \cdot \left(\rho(x, \sigma) F_\sigma(x) \right) = 0. \quad (5.6)$$

In the above formula we have a first order polynomial in λ and we have equality to zero for any value of λ if and only if the coefficients of the zero and first order terms are equal to zero separately:

$$\begin{cases} \nabla \cdot \left(\rho(x, \sigma) F_\sigma(x) \right) = 0, \\ \sum_{\sigma' \in \Gamma} \left(\rho(x, \sigma) r(\sigma, \sigma' | x) - \rho(x, \sigma') r(\sigma', \sigma | x) \right) = \nabla S(x) \cdot \left(\rho(x, \sigma) F_\sigma(x) \right). \end{cases} \quad (5.7)$$

The first equation, one for any fixed $\sigma \in \Gamma$, can be written as

$$\nabla \varphi(x, \sigma) \cdot F_\sigma(x) = -\nabla \cdot F_\sigma(x), \quad (5.8)$$

where we set $\varphi(x, \sigma) = \log \rho(x, \sigma)$ (here and below we suppose that $\rho(x, \sigma) > 0$ for all $(x, \sigma) \in \Omega \times \Gamma$ due to some mixing property of the system). Under the same assumption, the second equation, one for any fixed $\sigma \in \Gamma$, can be written in the equivalent form

$$\gamma(\sigma | x) - \gamma^+(\sigma | x) = \nabla S(x) \cdot F_\sigma(x). \quad (5.9)$$

Equation (5.8) is a non-homogeneous transport equation along the orbits of the vector fields F_σ . The important fact is that, as σ varies, these equations are uncoupled, hence one can easily integrate them. We distinguish between closed and open orbits.

Closed orbits: Let $\gamma \subseteq \Omega$ be a closed orbit of the vector field F_σ , let x_0 be any element of γ and let $x_\gamma(t)$ be the parametrization of γ such that $x_\gamma(0) = x_0$ and $\dot{x}_\gamma(t) = F_\sigma(x_\gamma(t))$ for all $t \in [0, T]$, where T is the period of the orbit (note that $x_\gamma(0) = x_\gamma(T) = x_0$). Given $x' \in \gamma$, let t' be the only time in $[0, T]$ such that $x' = x_\gamma(t')$. Then (5.8) implies that

$$\begin{aligned} \varphi(x', \sigma) - \varphi(x_0, \sigma) &= \int_0^{t'} \nabla \varphi(x_\gamma(s), \sigma) \cdot \dot{x}_\gamma(s) ds = \\ &= \int_0^{t'} \nabla \varphi(x_\gamma(s), \sigma) \cdot F_\sigma(x_\gamma(s)) ds = - \int_0^{t'} \nabla \cdot F_\sigma(x_\gamma(s)) ds. \end{aligned} \quad (5.10)$$

This implies that a function φ satisfying (5.8) can be constructed along γ if and only if the univalued condition

$$\int_0^T \nabla \cdot F_\sigma(x_\gamma(s)) ds = 0 \quad (5.11)$$

is satisfied. Moreover the values of φ on γ are uniquely determined from (5.10) once the initial condition $\varphi(x_0, \sigma)$ has been arbitrarily fixed.

Open orbits: Let $\gamma \subseteq \Omega$ be an open orbit of the vector field F_σ and consider $x_0 \in \gamma$. Let $x_\gamma(t)$ be a parametrization of γ such that $\dot{x}_\gamma(t) = F_\sigma(x_\gamma(t))$ and $x(0) = x_0$. Given $x' \in \gamma$,

let t' be the unique time such that $x_\gamma(t') = x'$. Then (5.10) continues to hold and we can determine the value of $\varphi(x', \sigma)$ for any $x' \in \gamma$ starting from the arbitrary initial condition $\varphi(x_0, \sigma)$.

Once determined $\rho(x, \sigma)$ by integration of the first group of equations in (5.7), we need to find a function S satisfying the second group of equations in (5.7). Let us call

$$D(x, \sigma) := \sum_{\sigma' \in \Gamma} \left(\rho(x, \sigma) r(\sigma, \sigma' | x) - \rho(x, \sigma') r(\sigma', \sigma | x) \right). \quad (5.12)$$

Then, the second group of equations in (5.7) reads

$$D(x, \sigma) = \nabla S(x) \cdot (\rho(x, \sigma) F_\sigma(x)), \quad \forall (x, \sigma) \in \Omega \times \Gamma. \quad (5.13)$$

This means that, for any $\sigma \in \Gamma$, $D(x, \sigma)$ is the directional derivative of S at x along the vector $\rho(x, \sigma) F_\sigma(x)$. In fact, given a vector $v \in \mathbb{R}^d$ the directional derivative of S along v at x is given by

$$\lim_{t \rightarrow 0} \frac{S(x + tv) - S(x)}{t} = \nabla S(x) \cdot v. \quad (5.14)$$

Let us assume that there exists $\Gamma(x) \subseteq \Gamma$ with the property that the vectors $\rho(x, \sigma) F_\sigma(x)$, $\sigma \in \Gamma(x)$, are linearly independent and satisfy

$$\text{Span} \{ \rho(x, \sigma) F_\sigma(x) \}_{\sigma \in \Gamma(x)} = \text{Span} \{ \rho(x, \sigma) F_\sigma(x) \}_{\sigma \in \Gamma} = \mathbb{R}^d, \quad (5.15)$$

where for generic vectors v_1, \dots, v_k in \mathbb{R}^d we write

$$\text{Span} \{ v_i \}_{i=1, \dots, k} := \left\{ v \in \mathbb{R}^d : v = \sum_{i=1}^k \lambda_i v_i, \lambda_i \in \mathbb{R} \right\}.$$

Note that (5.15) implies the identity $d = |\Gamma(x)|$ and that, since $\rho(x, \sigma) > 0$, (5.15) is equivalent to the condition

$$\text{Span} \{ F_\sigma(x) \}_{\sigma \in \Gamma(x)} = \text{Span} \{ F_\sigma(x) \}_{\sigma \in \Gamma} = \mathbb{R}^d. \quad (5.16)$$

Due to (5.15), for any $\sigma^* \notin \Gamma(x)$ there exist real numbers $c_\sigma(\sigma^*, x)$ such that

$$\rho(x, \sigma^*) F_{\sigma^*}(x) = \sum_{\sigma \in \Gamma(x)} c_\sigma(\sigma^*, x) \rho(x, \sigma) F_\sigma(x). \quad (5.17)$$

Let us recall a trivial consequence of (5.14): given vectors v, v_1, \dots, v_k such that $v = \sum_i c_i v_i$, it holds

$$\lim_{t \rightarrow 0} \frac{S(x + tv) - S(x)}{t} = \sum_i c_i \nabla S(x) \cdot v_i = \sum_i c_i \lim_{t \rightarrow 0} \frac{S(x + tv_i) - S(x)}{t}. \quad (5.18)$$

From (5.17) and (5.18) we get that a necessary condition for the existence of the function S is given by the family of identities

$$D(x, \sigma^*) = \sum_{\sigma \in \Gamma(x)} c_\sigma(\sigma^*, x) D(x, \sigma) \quad \forall \sigma^* \notin \Gamma(x). \quad (5.19)$$

We now derive a second necessary condition concerning D . Let $\{A_{i,\sigma}(x)\}_{i \in \{1, \dots, d\}}^{\sigma \in \Gamma(x)}$ be the $d \times d$ matrix, with rows labeled by the spatial dimensions and columns labeled by the chemical states in $\Gamma(x)$, defined as follows. The column with label σ is given by the vector

$\rho(x, \sigma)F_\sigma(x)$, i.e. $A_{i,\sigma}(x) = \rho(x, \sigma)F_\sigma(x) \cdot e_i$, where $(e_i, 1 \leq i \leq d)$ denotes the canonical basis of \mathbb{R}^d . This definition implies that

$$\rho(x, \sigma)F_\sigma(x) = \sum_{i=1}^d A_{i,\sigma}(x)e_i, \quad \forall \sigma \in \Gamma(x), \quad (5.20)$$

as well as

$$e_i = \sum_{\sigma \in \Gamma(x)} A_{\sigma,i}^{-1}(x) \rho(x, \sigma)F_\sigma(x), \quad \forall i : 1 \leq i \leq d. \quad (5.21)$$

The matrix $A^{-1}(x)$ is the inverse of the matrix $A(x)$ and has columns labeled by the spatial dimensions, and rows labeled by the chemical states in $\Gamma(x)$. Since $\{D(x, \sigma)\}_{\sigma \in \Gamma(x)}$ must correspond to directional derivatives of a function S on Ω , due to (5.18) and (5.21) it must be

$$\partial_{x_i} S(x) = \sum_{\sigma \in \Gamma(x)} A_{\sigma,i}^{-1}(x) D(x, \sigma). \quad (5.22)$$

Consider a closed curve $\gamma \subseteq \Omega$ with parametrization $\{x_\gamma(t)\}_{t \in [0, T]}$. Since γ is closed, it must be

$$0 = \int_0^T \nabla S(x_\gamma(s)) \cdot \dot{x}_\gamma(s) ds. \quad (5.23)$$

Using (5.22) the above identity becomes

$$0 = \int_0^T \sum_{i=1}^d \left(\sum_{\sigma \in \Gamma(x_\gamma(s))} A_{\sigma,i}^{-1}(x_\gamma(s)) D(x_\gamma(s), \sigma) \right) \dot{x}_{\gamma,i}(s) ds = \oint_\gamma \omega, \quad (5.24)$$

where ω is the differential form

$$\omega = \sum_{i=1}^d \left(\sum_{\sigma \in \Gamma(x)} A_{\sigma,i}^{-1}(x) D(x, \sigma) \right) dx_i. \quad (5.25)$$

The validity of condition (5.24) for any closed curve γ is equivalent to require that the differential form (5.25) is exact. When the domain Ω is simply connected, exactness of ω is equivalent to say that

$$\partial_{x_i} \left(\sum_{\sigma \in \Gamma(x)} A_{\sigma,j}^{-1}(x) D(x, \sigma) \right) = \partial_{x_j} \left(\sum_{\sigma \in \Gamma(x)} A_{\sigma,i}^{-1}(x) D(x, \sigma) \right), \quad \forall i \neq j. \quad (5.26)$$

We can now collect all our observations and reach a conclusion: conditions (5.15) and (5.19) together with the exactness of ω allow to determine a solution S of the second group of equations in (5.7), up to additive terms, as follows. Fix an arbitrary point $x^* \in \Omega$ and a corresponding arbitrary value $S(x^*)$. Given an arbitrary curve γ that starts in x^* and ends in $x \in \Omega$ (recall that for simplicity we have taken Ω connected), the value $S(x)$ is given by

$$S(x) = \int_\gamma \omega + S(x^*). \quad (5.27)$$

Due to the exactness of ω this value does not depend on the particular curve γ chosen. Note that by construction $dS = d\omega$, and therefore (5.22) is satisfied for any direction i . Due to (5.20), (5.21) and (5.18), this implies that $D(x, \sigma)$ is the directional derivative of S along the vector $\rho(x, \sigma)F_\sigma(x)$ at x , for any $x \in \Omega$ and for any $\sigma \in \Gamma(x)$. Due to condition (5.19) and to the additivity property (5.18), the same result extends also to states $\sigma \in \Gamma \setminus \Gamma(x)$. Hence, the function S satisfies the second group of equations in (5.7).

Above we have constructed solutions of (3.5) having the special form (5.1). To have that these solutions coincide with the invariant measures of the PDMP, we have to impose the boundary conditions (3.6) if Ω is a bounded domain in \mathbb{R}^d , or periodic boundary conditions in x if Ω is the d -dimensional torus. This has to be done, when possible, using the arbitrariness in the initial data in the above construction.

We end our general discussion with a remark. Since by definition (5.12) the sum $\sum_{\sigma \in \Gamma} D(x, \sigma)$ must be zero and since by (5.7) it holds $D(x, \sigma) = \nabla S(x) \cdot (\rho(x, \sigma) F_\sigma(x))$, it must be

$$\nabla S(x) \cdot \left(\sum_{\sigma \in \Gamma} \rho(x, \sigma) F_\sigma(x) \right) = 0. \quad (5.28)$$

In particular, the orbits of the vector field $\sum_{\sigma \in \Gamma} \rho(x, \sigma) F_\sigma(x)$ must lie inside the level curves of S .

5.2. Examples. We now exhibit solutions of (3.5) in specific examples by means of the above construction. The reader can easily check that our solutions satisfy the appropriate boundary conditions so that they correspond to the invariant measure of the PDMPs under consideration.

5.2.1. Interval. We review the PDMP of Subsection 4.1 by means of the general method described above. We keep the notation and assumptions already stated in Subsection 4.1. In particular, $\Omega = (a, b)$, F_1 has a unique orbit, which is open and exits from a , while F_0 has a unique orbit, which is open and exits from b . We fix an arbitrary point $x_* \in (a, b)$. Given $x(t)$ the solution of

$$\begin{cases} \dot{x} = F_1(x), \\ x(0) = x_*, \end{cases} \quad (5.29)$$

then due to (5.8) for any $x \in (a, b)$ the function $\varphi(x, 1) = \log \rho(x, 1)$ satisfies

$$\varphi(x, 1) = \phi(x_*) - \int_0^t \nabla \cdot F_1(x(s)) ds \quad (5.30)$$

where the time t is such that $x(t) = x$ and $\phi(x_*)$ is an arbitrary constant. Differentiating (5.29) we get

$$\frac{\ddot{x}(s)}{\dot{x}(s)} = \nabla \cdot F_1(x(s))$$

that inserted in (5.30) gives

$$\varphi(x, 1) = \phi(x_*) - \int_0^t \frac{d}{ds} (\log \dot{x}(s)) ds = \phi(x_*) + \log \frac{F_1(x_*)}{F_1(x)}.$$

The above identity and similar arguments applied to the vector field F_0 imply that

$$\begin{cases} \rho(x, 1) = e^{\phi(x_*) \frac{F_1(x_*)}{F_1(x)}}, \\ \rho(x, 0) = e^{\psi(x_*) \frac{F_0(x_*)}{F_0(x)}}, \end{cases} \quad (5.31)$$

where also $\psi(x_*)$ is an arbitrary constant. It remains now to determine the function S and afterwards to fix the arbitrary constants. Taking $\Gamma(x) = \{1\}$ for any $x \in \Omega$, condition (5.16) is satisfied. Due to (5.31), we can express the constant $c_1(0, x)$ in (5.17) as

$$c_1(0, x) = \frac{\rho(x, 0) F_0(x)}{\rho(x, 1) F_1(x)} = \frac{e^{\psi(x_*) F_0(x_*)}}{e^{\phi(x_*) F_1(x_*)}}. \quad (5.32)$$

Since in addition $D(x, 0) = -D(x, 1)$, condition (5.19) is satisfied if and only if $c_1(0, x) \equiv -1$. To this aim we take $e^{\psi(x_*)} = -1/F_0(x_*)$ and $e^{\phi(x_*)} = 1/F_1(x_*)$. By this choice, the differential form (5.25) is given by

$$\omega = \frac{D(x, 1)}{\rho(x, 1)F_1(x)} dx = \left(\frac{r(0, 1|x)}{F_0(x)} + \frac{r(1, 0|x)}{F_1(x)} \right) dx. \quad (5.33)$$

The form ω is trivially exact, being a 1D form on a simply connected domain. Then, by formula (5.27) and the previous computations, we get (4.3) as a special case of (5.1).

5.2.2. 1D torus. In the case of the 1D torus discussed in Subsection 4.2, we have $\Omega = \mathbb{R}/\mathbb{Z}$ and both F_0 and F_1 have a closed orbit that coincide with Ω . In both cases the univalued condition (5.11) is satisfied due to the fact that on the periodic orbit $x(t)$ solution of $\dot{x} = F_i(x)$ with period T we have

$$\int_0^T \nabla \cdot F_i(x(s)) ds = \int_0^T \frac{d}{ds} (\log \dot{x}(s)) ds = 0.$$

We can repeat all the arguments and computations of the case $\Omega = (a, b)$. The only exception is that now the form ω given by (5.33) is not automatically exact, since Ω is not simply connected. The requirement that $\oint_{\Omega} \omega = 0$ is exactly the equilibrium condition (4.9). The final result coincides with (4.18).

5.2.3. Triangular domain. Let us now discuss a simple but non trivial example in dimension $d = 2$ of a PDMP with an invariant measure of the form (5.1). Let $\Omega \subseteq \mathbb{R}^2$ be the open triangle with vertices $(0, 0)$, $(1, 0)$, $(0, 1)$ and let (x, y) denote a generic element of Ω . The set of chemical states is $\Gamma = \{1, 2, 3\}$. The vector fields associated to the chemical states are obtained from the gradients of quadratic potentials centered at the vertices of the triangle. More precisely

$$\begin{cases} F_1(x, y) = -\frac{1}{2} \nabla (x^2 + y^2) = (-x, -y), \\ F_2(x, y) = -\frac{1}{2} \nabla ((x-1)^2 + y^2) = (1-x, -y), \\ F_3(x, y) = -\frac{1}{2} \nabla (x^2 + (y-1)^2) = (-x, 1-y). \end{cases}$$

All the orbits of the above vector fields are open and condition (2.12) is satisfied. Moreover the orbits of the vector fields F_i exit from $\partial\Omega_i^+ \subset \partial\Omega$, where $\partial\Omega_1^+$ is the segment with extrema $(0, 1)$ and $(1, 0)$; $\partial\Omega_2^+$ is the segment with extrema $(0, 0)$ and $(0, 1)$; $\partial\Omega_3^+$ is the segment with extrema $(0, 0)$ and $(1, 0)$. Let us determine the function $\varphi(x, y, 1) = \log \rho(x, y, 1)$ by means of the discussion following (5.8). To this aim, we observe that given $(x, y) \in \Omega$ the path $(x(t), y(t)) := (e^{-t}, e^{-t}y/x)$ satisfies

$$\begin{cases} (\dot{x}(t), \dot{y}(t)) = F_1(x(t), y(t)), & \forall t \geq t_0, \\ (x(t_0), y(t_0)) = (x/(x+y), y/(x+y)) \in \partial\Omega_1^+, \\ (x(t_1), y(t_1)) = (x, y), \end{cases}$$

where $t_0 := \log((x+y)/x)$ and $t_1 := \log(1/x)$. In particular, the above path parameterized by $t \geq t_0$ is an orbit of F_1 exiting from $\partial\Omega_1^+$ and passing through the point (x, y) . Fixed an arbitrary function $\phi_1 : (0, 1) \rightarrow \mathbb{R}$ we obtain using (5.10)

$$\varphi(x, y, 1) - \phi_1\left(\frac{x}{x+y}\right) = 2 \int_{\log \frac{x+y}{x}}^{\log \frac{1}{x}} dt = -2 \log(x+y),$$

so that $\rho(x, y, 1) = \frac{e^{\phi_1(\frac{x}{x+y})}}{(x+y)^2}$. Note that this can be rewritten as $\rho(x, y, 1) = a_1(x/(x+y))/x^2$ for a suitable function $a_1 : (0, 1) \rightarrow \mathbb{R}$. In conclusion, by similar arguments, we get that

$$\begin{cases} \rho(x, y, 1) = a_1 \left(\frac{x}{x+y} \right) \frac{1}{x^2}, \\ \rho(x, y, 2) = a_2 \left(\frac{y}{1-x} \right) \frac{1}{y^2}, \\ \rho(x, y, 3) = a_3 \left(\frac{x}{1-y} \right) \frac{1}{x^2}, \end{cases} \quad (5.34)$$

for positive functions a_1, a_2, a_3 , which can be chosen arbitrarily. Note that the point $(0, y/(1-x))$ is the exit point in $\partial\Omega_2^+$ of the F_2 -orbit passing through the point $(x, y) \in \Omega$, while $(x/(1-y), 0)$ is the exit point in $\partial\Omega_3^+$ of the F_3 -orbit passing through the point $(x, y) \in \Omega$.

In order to determine the function S of (5.1), for any $(x, y) \in \Omega$ we take $\Gamma(x, y) = \{2, 3\}$. Trivially condition (5.16) is satisfied. Moreover, we can compute $c_2(1, x, y)$ and $c_3(1, x, y)$ of (5.17):

$$\begin{cases} c_2(1, x, y) = \frac{x}{x+y-1} \frac{\rho(x, y, 1)}{\rho(x, y, 2)}, \\ c_3(1, x, y) = \frac{y}{x+y-1} \frac{\rho(x, y, 1)}{\rho(x, y, 3)}. \end{cases} \quad (5.35)$$

At this point, the check of condition (5.19) depends strongly from the form of the rates $r(\cdot, \cdot | x, y)$. Indeed, omitting the dependence from the point (x, y) (for the sake of simplicity) condition (5.19) becomes

$$\begin{aligned} r(1, 2) + r(1, 3) - \frac{\rho(2)}{\rho(1)} r(2, 1) - \frac{\rho(3)}{\rho(1)} r(3, 1) = \\ \frac{x}{x+y-1} \left[r(2, 1) + r(2, 3) - \frac{\rho(1)}{\rho(2)} r(1, 2) - \frac{\rho(3)}{\rho(2)} r(3, 2) \right] + \\ \frac{y}{x+y-1} \left[r(3, 1) + r(3, 2) - \frac{\rho(1)}{\rho(3)} r(1, 3) - \frac{\rho(2)}{\rho(3)} r(2, 3) \right]. \end{aligned} \quad (5.36)$$

As the reader can easily check, the above identity is automatically satisfied for all kind of jump rates if

$$\frac{\rho(1)}{\rho(3)} = \frac{1-x-y}{y}, \quad \frac{\rho(2)}{\rho(3)} = \frac{x}{y}, \quad \frac{\rho(1)}{\rho(2)} = \frac{1-x-y}{x}. \quad (5.37)$$

In order to satisfy the above identities it is enough to take a_1, a_2, a_3 in (5.34) as $a_i(u) = \frac{u}{1-u}$. By this choice, (5.34) reads

$$\begin{cases} \rho(x, y, 1) = 1/(xy), \\ \rho(x, y, 2) = 1/[y(1-x-y)], \\ \rho(x, y, 3) = 1/[x(1-x-y)]. \end{cases} \quad (5.38)$$

It remains now to compute the form ω given by (5.25), check when it is exact and afterwards check the boundary condition (3.6). First we observe that

$$A(x, y) = \frac{1}{1-x-y} \begin{pmatrix} \frac{1-x}{y} & -1 \\ -1 & \frac{1-y}{x} \end{pmatrix}, \quad A^{-1}(x, y) = \begin{pmatrix} y(1-y) & xy \\ xy & x(1-x) \end{pmatrix}.$$

Therefore

$$\omega = [y(1-y)D(x, y, 2) + xyD(x, y, 3)] dx + [xyD(x, y, 2) + x(1-x)D(x, y, 3)] dy.$$

We have

$$\omega = B(x, y)dx + C(x, y)dy$$

where (omitting the dependence on (x, y) for simplicity)

$$\begin{aligned} B(x, y) &= \frac{1-y}{1-x-y}r(2, 1) - \frac{1-y}{x}r(1, 2) + \frac{y}{1-x-y}r(3, 1) - r(1, 3) + r(2, 3) - \frac{y}{x}r(3, 2), \\ C(x, y) &= \frac{1-x}{1-x-y}r(3, 1) - \frac{1-x}{y}r(1, 3) + \frac{x}{1-x-y}r(2, 1) - r(1, 2) + r(3, 2) - \frac{x}{y}r(2, 3). \end{aligned}$$

Note that $C(x, y)$ can be obtained from $B(x, y)$ by exchanging x with y and 2 with 3.

If, motivated by the geometric symmetries of Ω , we assume that

$$r(1, 2|x, y) = r(1, 3|y, x), \quad r(2, 1|x, y) = r(3, 1|y, x), \quad r(2, 3|x, y) = r(3, 2|y, x)$$

then

$$\omega = B(x, y)dx + B(y, x)dy.$$

In this case, since Ω is simply connected, ω is exact if and only if $\partial_y B(a, b) = \partial_y B(b, a)$ (cf. (5.26)), i.e the function $\partial_y B$ is symmetric.

Let us discuss an example, where the above condition is satisfied. We take $r(\sigma, \sigma'|x, y) = 1$ for all $\sigma \neq \sigma'$. Then one easily compute the above $B(x, y)$ and $C(x, y)$, getting

$$\omega = \frac{2x+y-1}{x(1-x-y)}dx + \frac{2y+x-1}{y(1-x-y)}dy, \quad (5.39)$$

which is exact since the domain Ω is simply connected and condition (5.26) is satisfied. Integrating the form ω as in (5.27), we obtain up to an arbitrary constant

$$S(x, y) = \int_{\gamma} \omega = -\log x - \log y - \log(1-x-y). \quad (5.40)$$

By collecting our results (5.38) and (5.40), we obtain that the invariant measure is of the form (5.1) and that

$$\begin{aligned} \rho_{\lambda} &= \left(\rho_{\lambda}(x, y, 1), \rho_{\lambda}(x, y, 2), \rho_{\lambda}(x, y, 3) \right) = \\ &= c(\lambda) \left(x^{\lambda-1}y^{\lambda-1}(1-x-y)^{\lambda}, x^{\lambda}y^{\lambda-1}(1-x-y)^{\lambda-1}, x^{\lambda-1}y^{\lambda}(1-x-y)^{\lambda-1} \right). \end{aligned}$$

Above, $c(\lambda)$ is the normalization constant, which is well-defined as the reader can easily check. Finally, we observe that the above invariant measure satisfies the boundary condition (3.6).

Note that, due to (5.34), (3.6) can be satisfied only if S diverges to $-\infty$ when approaching the boundary of the triangle Ω . This is a strong restriction. For example, if we take $r(3, 2|x, y) = r(2, 3|x, y) = 0$, $r(2, 1|x, y) = r(3, 1|x, y) = 1-x-y$, $r(1, 2|x, y) = r(1, 3|y, x) = x$, we obtain that $\omega = dS$ where S is a constant function, thus leading to a solution of the stationary equations (3.5), but not satisfying the boundary condition (3.6).

5.2.4. 2D torus. We take $\Omega = \mathbb{R}^2/\mathbb{Z}^2$ and $\Gamma = \{0, 1\}$. We call (x, y) a generic element of Ω and choose vector fields

$$\begin{cases} F_0(x, y) = (f(x, y), 0), \\ F_1(x, y) = (0, g(x, y)), \end{cases}$$

where f and g are regular functions which never vanish on Ω . The chemical part of the generator is determined by the transition rates $r(i, i-1|x, y)$ $i = 0, 1$. The first group of equations in (5.7) can be easily solved:

$$\begin{cases} \rho(x, y, 0) = \frac{\phi(y)}{f(x, y)}, \\ \rho(x, y, 1) = \frac{\tilde{\phi}(x)}{g(x, y)}; \end{cases}$$

where ϕ and $\tilde{\phi}$ are arbitrary functions. Moreover we have that

$$A^{-1}(x, y) = \begin{pmatrix} \frac{1}{\phi(y)} & 0 \\ 0 & \frac{1}{\phi(x)} \end{pmatrix},$$

hence ω can be written as

$$\omega = \left(\frac{r(0, 1|x, y)}{f(x, y)} - \frac{\tilde{\phi}(x)r(1, 0|x, y)}{\phi(y)g(x, y)} \right) dx + \left(\frac{r(1, 0|x, y)}{g(x, y)} - \frac{\phi(y)r(0, 1|x, y)}{\tilde{\phi}(x)f(x, y)} \right) dy. \quad (5.41)$$

Fix arbitrary points $x^*, y^* \in [0, 1]$ and consider the associated fundamental cycles on Ω

$$\begin{cases} \gamma^1(t) = (t, y^*) & t \in [0, 1], \\ \gamma^2(t) = (x^*, t) & t \in [0, 1]. \end{cases}$$

The exactness of (5.41) is equivalent to impose conditions (5.26) with the additional conditions

$$\oint_{\gamma^1} \omega = \oint_{\gamma^2} \omega = 0. \quad (5.42)$$

If we call $H(x, y) = \phi(y)r(0, 1|x, y)/f(x, y)$ and $G(x, y) = \tilde{\phi}(x)r(1, 0|x, y)/g(x, y)$, then we can write ω as

$$\omega = \frac{H(x, y) - G(x, y)}{\phi(y)} dx + \frac{G(x, y) - H(x, y)}{\tilde{\phi}(x)} dy,$$

hence the above exactness conditions become

$$\begin{cases} \int_0^1 H(x^*, y) dy = \int_0^1 G(x^*, y) dy, \\ \int_0^1 H(x, y^*) dx = \int_0^1 G(x, y^*) dx, \\ \partial_x \left(\frac{G(x, y) - H(x, y)}{\phi(y)} \right) = \partial_y \left(\frac{H(x, y) - G(x, y)}{\tilde{\phi}(x)} \right). \end{cases}$$

Examples of rates $r(i, i-1|x, y)$ satisfying these conditions can be easily constructed.

5.2.5. Square domain. We consider the open square $\Omega \subseteq \mathbb{R}^2$ with vertices $(0, 0)$, $(0, 1)$, $(1, 0)$ and $(1, 1)$. The chemical states are $\Gamma = \{0, 1, 2, 3\}$ with associated vector fields

$$\begin{aligned} F_0(x, y) &= (-x, -y), & F_1(x, y) &= (1-x, -y), \\ F_2(x, y) &= (-x, 1-y), & F_3(x, y) &= \alpha(1-x, 1-y), \end{aligned}$$

where α is a positive parameter and (x, y) is a generic element of Ω . We choose the jump rates as

$$\begin{aligned} r(0, 1|x, y) &= r(0, 2|y, x) = q(x, y), & r(1, 0|x, y) &= r(2, 0|y, x) = r(x, y), \\ r(1, 3|x, y) &= r(2, 3|y, x) = Q(x, y), & r(3, 1|x, y) &= r(3, 2|y, x) = R(x, y), \end{aligned}$$

where q, r, Q and R are arbitrary positive functions and moreover $r(1, 2|x, y) = r(2, 1|x, y) = 0$.

Proceeding as in the previous examples we obtain a solution of the form (5.1) if we require that the rates satisfy the following relations: there exists a function $G(x, y)$ such that

$$\begin{cases} q(x, y) - Q(x, y) = G(x, y)x, \\ r(x, y) - \frac{R(x, y)}{\alpha} = G(x, y)(1 - x). \end{cases}$$

and there exists a symmetric function $s(x, y)$ and a function ϕ such that

$$xR(x, y) - \alpha(1 - x)Q(x, y) = \alpha x(1 - x) \left(\int_z^y du s(x, u) + \phi(x) \right),$$

where $z \in (0, 1)$. Under the above conditions we have a solution of the form (5.1) with

$$S(x, y) = \int_z^x dw \int_z^y du s(w, u) + \int_z^x dw \phi(w) + \int_z^y du \phi(u),$$

and

$$\begin{aligned} \rho(x, y, 0) &= \frac{1}{xy}, & \rho(x, y, 1) &= \frac{1}{y(1-x)}, \\ \rho(x, y, 2) &= \frac{1}{x(1-y)}, & \rho(x, y, 3) &= \frac{1}{\alpha(1-x)(1-y)}. \end{aligned}$$

Boundary conditions (3.6) are not necessarily satisfied.

6. AVERAGING AND LARGE DEVIATION PRINCIPLES IN THE HIGH FREQUENCY LIMIT

In this section we study the asymptotic behavior of our PDMPs and the corresponding time-reversed versions as the parameter λ diverges to infinity. By this limit, the frequency of chemical jumps diverges and the timescale of chemical jumps becomes infinitesimal w.r.t. the relaxation time of the mechanical state. Below, we recall some rigorous results derived in [12], where the interested reader can find a more detailed discussion.

In order to describe the asymptotic behavior of the system and analyze deviations from it, we need to specify carefully both the limit procedure and the involved spaces. Given a time interval $[0, T]$, a trajectory $\{x(t)\}_{t \in [0, T]}$ of the mechanical variable is a continuous function $x : [0, T] \rightarrow \Omega$. It is then natural to consider the mechanical trajectories as elements of the path space $C([0, T], \Omega)$ endowed with the topology induced by the sup norm. A chemical trajectory $\{\sigma(t)\}_{t \in [0, T]}$ is an element of the Skorokhod space $D([0, T], \Gamma)$ of right continuous functions having left limit and taking values in $\Gamma = \{\sigma_1, \dots, \sigma_{|\Gamma|}\}$. To a chemical trajectory we associate the following time-dependent d -dimensional vector

$$\{\sigma(t)\}_{t \in [0, T]} \rightarrow \{\chi(t)\}_{t \in [0, T]} = \left\{ (\chi_{\sigma_1}(t), \dots, \chi_{\sigma_{|\Gamma|}}(t)) \right\}_{t \in [0, T]},$$

where

$$\chi_{\sigma}(t) = \begin{cases} 1 & \text{if } \sigma(t) = \sigma, \\ 0 & \text{if } \sigma(t) \neq \sigma. \end{cases}$$

We denote by $\mathcal{M}([0, T])$ the space of nonnegative finite measures on the interval $[0, T]$, endowed of the weak convergence topology. Namely, $\mu_n \rightarrow \mu$ in $\mathcal{M}([0, T])$ if and only if $\int_0^T f(t) \mu_n(dt) \rightarrow \int_0^T f(t) \mu(dt)$ for all continuous functions f on $[0, T]$. Then we isolate the subspace $\mathcal{M}_0([0, T]) \subset \mathcal{M}([0, T])$ given by the measures that are absolutely continuous w.r.t. the Lebesgue measure. We can interpret $\{\chi(t)\}_{t \in [0, T]}$ as an element of the cartesian product $\mathcal{M}_0([0, T])^\Gamma$ by identifying $\{\chi_{\sigma}(t)\}_{t \in [0, T]}$ with the measure $\chi_{\sigma}(t)dt$. If our PDMP

starts in the state (x_0, σ_0) , we can think its evolution $\{x(t), \chi(t)\}_{t \in [0, T]}$ as an element of following subset \mathcal{Y}_{x_0} of $C([0, T], \Omega) \times \mathcal{M}_0([0, T])^\Gamma$:

$$\mathcal{Y}_{x_0} = \left\{ \{x(t), \chi(t)\}_{t \in [0, T]} \in C([0, T], \Omega) \times \mathcal{M}_0([0, T])^\Gamma : \right. \\ \left. \sum_{\sigma \in \Gamma} \chi_\sigma(t) = 1 \text{ a.e.}, \ x(t) = x_0 + \int_0^t \sum_{\sigma \in \Gamma} \chi_\sigma(s) F_\sigma(x(s)) ds \right\}. \quad (6.1)$$

Above, as in the rest of the paper, we write $\{x(t), \chi(t)\}_{t \in [0, T]}$ instead of $\{(x(t), \chi(t))\}_{t \in [0, T]}$ in order to simplify the notation. Moreover, in the above formula and hereafter we identify measures in $\mathcal{M}_0([0, T])$ with their corresponding densities. It can be proved (cf. [12]) that \mathcal{Y}_{x_0} is a compact subspace of $C[0, T] \times \mathcal{M}[0, T]^\Gamma$, and its topology can be derived from the metric d defined as

$$d(\{x(t), \chi(t)\}_{t \in [0, T]}, \{\bar{x}(t), \bar{\chi}(t)\}_{t \in [0, T]}) = \\ \sup_{t \in [0, T]} |x(t) - \bar{x}(t)| + \sum_{\sigma \in \Gamma} \sup_{0 \leq t \leq T} \left| \int_0^t [\chi_\sigma(s) - \bar{\chi}_\sigma(s)] ds \right|. \quad (6.2)$$

Moreover, in [12] we prove the following law of large numbers. Given $(x, \sigma) \in \Omega \times \Gamma$, we define the mean vector field $\bar{F}(x)$ as the average with respect to the quasistationary measure $\mu(\cdot|x)$ of the fields $F_\sigma(x)$:

$$\bar{F}(x) = \sum_{\sigma \in \Gamma} \mu(\sigma|x) F_\sigma(x). \quad (6.3)$$

Given the initial state (x_0, σ_0) , we call $\{x^*(t), \chi^*(t)\}_{t \in [0, T]}$ the unique element of \mathcal{Y}_{x_0} such that

$$\begin{cases} \dot{x}^*(t) = \bar{F}(x^*(t)), \\ x^*(0) = x_0, \\ \chi_\sigma^*(t) = \mu(\sigma|x^*(t)). \end{cases} \quad (6.4)$$

Then, the following law of large numbers holds:

$$\lim_{\lambda \rightarrow \infty} \mathbb{P}_{x_0, \sigma_0}^\lambda \left[d(\{x(t), \chi(t)\}_{t \in [0, T]}, \{x^*(t), \chi^*(t)\}_{t \in [0, T]}) > \delta \right] = 0, \quad \forall \delta > 0, \quad (6.5)$$

where the law $\mathbb{P}_{x_0, \sigma_0}^\lambda$ of the PDMP starting at (x_0, σ_0) and having parameter λ is thought of as a probability distribution on \mathcal{Y}_{x_0} . Above $\{x(t), \chi(t)\}_{t \in [0, T]}$ denotes a typical element of \mathcal{Y}_{x_0} . Finally, we point out that the limit element $\{x^*(t), \chi^*(t)\}_{t \in [0, T]}$ is independent from the initial chemical state σ_0 .

The above law of large numbers is a typical example of *Averaging Principle*. Indeed, we are dealing with a stochastic dynamical systems with fully-coupled fast and slow variables. In the high frequency limit, the fast variables χ average according to the local quasistationary measure as the slow variables x would be frozen, while the slow variables x feel the averaged vector field \bar{F} .

We briefly illustrate a *Large Deviation Principle*, where the probability of deviations from the above law of large numbers is computed on exponential scale. For precise statements and rigorous proofs we refer to [12], while we keep here the exposition at a more heuristic level. We are interested in the exponential probability rate of rare events, namely we look for a functional $J_{[0, T]}$ on \mathcal{Y}_{x_0} such that, for any fixed path $\{\hat{x}(t), \hat{\chi}(t)\} \in \mathcal{Y}_{x_0}$, it

holds

$$\mathbb{P}_{x_0, \sigma_0}^\lambda \left(\{x(t), \chi(t)\}_{t \in [0, T]} \approx \{\hat{x}(t), \hat{\chi}(t)\}_{t \in [0, T]} \right) \sim e^{-\lambda J_{[0, T]}(\{\hat{x}(t), \hat{\chi}(t)\}_{t \in [0, T]})}. \quad (6.6)$$

In the above formula, $\{x(t), \chi(t)\}_{t \in [0, T]}$ is a generic element of \mathcal{Y}_{x_0} , the symbol \approx means closeness in the metric of \mathcal{Y}_{x_0} and finally \sim means asymptotic logarithmic equivalence in the limit of diverging λ . The functional $J_{[0, T]}$ is called the rate functional.

For our PDMPs such a functional exists and has a variational representation. In order to describe it, we fix some notation. We denote by W the set of pairs

$$W := \{(\sigma, \sigma') \in \Gamma \times \Gamma : \sigma \neq \sigma'\}.$$

Given a point $x \in \Omega$ and a vector $\chi \in [0, 1]^\Gamma$, we define

$$j(x, \chi) := \sup_{z \in (0, \infty)^\Gamma} \sum_{(\sigma, \sigma') \in W} \chi_\sigma r(\sigma, \sigma' | x) \left[1 - \frac{z_{\sigma'}}{z_\sigma} \right]. \quad (6.7)$$

Then the rate functional $J_{[0, T]} : \mathcal{Y}_{x_0} \rightarrow [0, \infty)$ is given by

$$J_{[0, T]}(\{x(t), \chi(t)\}_{t \in [0, T]}) := \int_0^T j(x(t), \chi(t)) dt. \quad (6.8)$$

Note that the above functional does not depend on σ_0 , but depends on x_0 since its domain is given by \mathcal{Y}_{x_0} .

If, given $x \in \Omega$, the chemical part $L_c[x]$ of the generator is reversible w.r.t. the quasi-stationary measure $\mu(\sigma | x)$, then one can solve the variational problem (6.7) (see [12] for details) getting:

$$j(x, \chi) = \sum_{\sigma} \gamma(\sigma | x) \chi_\sigma - \sum_{(\sigma, \sigma') \in W} \sqrt{\frac{\mu(\sigma | x)}{\mu(\sigma' | x)}} r(\sigma, \sigma' | x) \sqrt{\chi_\sigma} \sqrt{\chi_{\sigma'}}. \quad (6.9)$$

We know that the above condition is always satisfied if $|\Gamma| = 2$. Writing $\Gamma = \{0, 1\}$ one easily computes $j(\sigma, \chi)$ as

$$j(x, \chi) = \left(\sqrt{\chi_0 r(0, 1 | x)} - \sqrt{\chi_1 r(1, 0 | x)} \right)^2. \quad (6.10)$$

6.1. LDP for the mechanical state. It is natural to analyze the statistical behavior of the mechanical variables alone, since often the chemical variables remain hidden to direct observations. To this aim, by means of the contraction principle [11], one can derive the LDP rate functional $J_{[0, T]}^m : C([0, T], \Omega) \rightarrow [0, \infty]$ for the mechanical variables from the joint (chemical and mechanical) rate functional $J_{[0, T]}$ defined above. In particular, given an element $\{\hat{x}(t)\}_{t \in [0, T]} \in C([0, T], \Omega)$, for each initial state (x_0, σ_0) it holds

$$\mathbb{P}_{x_0, \sigma_0}^\lambda \left(\{x(t)\}_{t \in [0, T]} \approx \{\hat{x}(t)\}_{t \in [0, T]} \right) \sim e^{-\lambda J_{[0, T]}^m(\{\hat{x}(t)\}_{t \in [0, T]})},$$

where

$$J_{[0, T]}^m(\{x(t)\}_{t \in [0, T]}) = \inf_{\{\chi(t)\}_{t \in [0, T]} : \{x(t), \chi(t)\}_{t \in [0, T]} \in \mathcal{Y}_{x_0}} J_{[0, T]}(\{x(t), \chi(t)\}_{t \in [0, T]}). \quad (6.11)$$

Above, we have used the convention that the infimum over the empty set is defined as $+\infty$. From expression (6.8) we obtain that the functional $J_{[0, T]}^m : C([0, T], \Omega) \rightarrow [0, \infty]$

equals

$$J_{[0,T]}^m(\{x(t)\}_{t \in [0,T]}) = \begin{cases} \int_0^T j_m(x(t), \dot{x}(t)) dt & \text{if } x(\cdot) \in \mathcal{Y}_{x_0}^m, \\ +\infty & \text{otherwise,} \end{cases} \quad (6.12)$$

where

$$\mathcal{Y}_{x_0}^m := \left\{ \{x(t)\}_{t \in [0,T]} : \exists \{\chi(t)\}_{t \in [0,T]} \text{ s.t. } \{x(t), \chi(t)\}_{t \in [0,T]} \in \mathcal{Y}_{x_0} \right\}.$$

and the density $j_m(x, \dot{x})$ is given by

$$j_m(x, \dot{x}) = \inf_{\{\chi: \dot{x} = \sum_{\sigma} \chi_{\sigma} F_{\sigma}(x)\}} j(x, \chi). \quad (6.13)$$

In the above formula, χ varies among vectors in $[0, 1]^{\Gamma}$ such that $\sum_{\sigma} \chi_{\sigma} = 1$.

In general an explicit computation of j_m depends on the specific model we are dealing with. In formula (6.13) we are minimizing over all possible convex decompositions of the vector \dot{x} with respect to the collection of vectors $\{F_{\sigma}(x)\}_{\sigma \in \Gamma}$. A special case is when for any $x \in \Omega$ the collection of vectors $\{F_{\sigma}(x)\}_{\sigma \in \Gamma}$ are the vertices of a simplex, i.e. the vectors $\{F_{\sigma_j} - F_{\sigma_1} : 2 \leq j \leq |\Gamma|\}$ are independent (writing $\Gamma = \{\sigma_j : 1 \leq j \leq |\Gamma|\}$). In this case if the vector \dot{x} belong to $\mathcal{C}(\{F_{\sigma}(x)\}_{\sigma \in \Gamma})$, where the symbol $\mathcal{C}(\cdot)$ denotes the *convex hull*, then there exists a unique probability measure on Γ , $\chi^F(\dot{x})$, such that $\dot{x} = \sum_{\sigma} \chi_{\sigma}^F(\dot{x}) F_{\sigma}(x)$. The $\chi^F(\dot{x})$ are called the *barycentric coordinates* of \dot{x} with respect to the collection of vectors $\{F_{\sigma}(x)\}_{\sigma \in \Gamma}$. The upper index F indicates the dependence on the vector fields, the dependence on x is understood. When $\dot{x} \notin \mathcal{C}(\{F_{\sigma}(x)\}_{\sigma \in \Gamma})$ then the infimum in (6.13) is over an empty set and we obtain

$$j_m(x, \dot{x}) = \begin{cases} j(x, \chi^F(\dot{x})) & \text{if } \dot{x} \in \mathcal{C}(\{F_{\sigma}(x)\}_{\sigma \in \Gamma}), \\ +\infty & \text{otherwise.} \end{cases} \quad (6.14)$$

We will compute the rate density $j_m(x, \dot{x})$ in specific examples in the next section.

6.2. LDP for the time-reversed process. Since the adjoint (time-reversed) process of our PDMP is again a PDMP with reversed vector fields, the space on which it is natural to study the adjoint process and its limiting behavior is

$$\mathcal{Y}_{x_0}^+ = \left\{ \{x(t), \chi(t)\}_{t \in [0,T]} \in C([0,T], \Omega) \times \mathcal{M}_0([0,T])^{\Gamma} : \sum_{\sigma \in \Gamma} \chi_{\sigma}(t) = 1 \text{ a.e., } x(t) = x_0 - \int_0^t \sum_{\sigma \in \Gamma} \chi_{\sigma}(s) F_{\sigma}(x(s)) ds \right\}. \quad (6.15)$$

For models having invariant measure of the form (5.1), the rates r^+ of the adjoint process do not depend on λ so that a LDP for the adjoint process can be obtained using again the results of [12]:

$$\mathbb{P}_{x_0, \sigma_0}^{\lambda, +} \left(\{x(t), \chi(t)\}_{t \in [0,T]} \approx \{\hat{x}(t), \hat{\chi}(t)\}_{t \in [0,T]} \right) \sim e^{-\lambda J_{[0,T]}^+ (\{\hat{x}(t), \hat{\chi}(t)\}_{t \in [0,T]})}, \quad (6.16)$$

where

$$J_{[0,T]}^+ (\{x(t), \chi(t)\}_{t \in [0,T]}) := \int_0^T j^+(x(t), \chi(t)) dt, \\ j^+(x, \chi) := \sup_{z \in (0, \infty)^{\Gamma}} \sum_{(\sigma, \sigma') \in W} \chi_{\sigma} r^+(\sigma, \sigma' | x) \left[1 - \frac{z_{\sigma'}}{z_{\sigma}} \right]. \quad (6.17)$$

In the above formula $\mathbb{P}_{x_0, \sigma_0}^{\lambda, +}$ is the probability measure on $\mathcal{Y}_{x_0}^+$ induced by the adjoint process with parameter λ and initial condition (x_0, σ_0) . Remember that in this case the rates r^+ in (6.17) are related to the rates r of the direct model from (5.2).

Let us assume now, as done for (6.9), that for all $x \in \Omega$ the chemical part $L_c[x]$ of the direct generator is reversible w.r.t. the quasistationary measure $\mu(\cdot|x)$. Then we know that the same property holds for the adjoint process with $\mu(\cdot|x)$ replaced by $\mu^+(\cdot|x)$. In this case, similarly to (6.9), we get

$$j^+(x, \chi) = \sum_{\sigma} \gamma^+(\sigma|x) \chi_{\sigma} - \sum_{(\sigma, \sigma') \in W} \sqrt{\frac{\mu^+(\sigma|x)}{\mu^+(\sigma'|x)}} r^+(\sigma, \sigma'|x) \sqrt{\chi_{\sigma}} \sqrt{\chi_{\sigma'}}. \quad (6.18)$$

Recalling relations (5.2) and (5.3) we obtain that

$$j^+(x, \chi) = \sum_{\sigma} \gamma^+(\sigma|x) \chi_{\sigma} - \sum_{(\sigma, \sigma') \in W} \sqrt{\frac{\mu(\sigma|x)}{\mu(\sigma'|x)}} r(\sigma, \sigma'|x) \sqrt{\chi_{\sigma}} \sqrt{\chi_{\sigma'}}. \quad (6.19)$$

As the reader can check, the proof of the LDP in [12] remains valid for PDMPs with λ -dependent rates $r(\sigma, \sigma', \lambda|x)$ obtained as perturbation of λ -independent rates, i.e. $r(\sigma, \sigma', \lambda|x) = r(\sigma, \sigma'|x)(1 + o(1))$. Hence, the above result (6.16) can be extended to more general processes with invariant measures not of the form (5.1). We will discuss an example in the next section.

Let us now consider the LD rate functional $J_{[0, T]}^{m, +} : C([0, T], \Omega) \rightarrow [0, \infty]$ for the evolution of the mechanical state in the adjoint process (dropping the above the reversibility assumption). It has the form

$$J_{[0, T]}^{m, +}(\{x(t)\}_{t \in [0, T]}) = \begin{cases} \int_0^T j_m^+(x(t), \dot{x}(t)) dt & \text{if } x(\cdot) \in \mathcal{Y}_{x_0}^{m, +}, \\ +\infty & \text{otherwise,} \end{cases} \quad (6.20)$$

where, similarly to $\mathcal{Y}_{x_0}^m$, the space $\mathcal{Y}_{x_0}^{m, +}$ is defined as the mechanical projection of $\mathcal{Y}_{x_0}^+$, while the density $j_m^+(x, \dot{x})$ is given by

$$j_m^+(x, \dot{x}) = \inf_{\{\chi: \dot{x} = -\sum_{\sigma} \chi_{\sigma} F_{\sigma}(x)\}} j^+(x, \chi). \quad (6.21)$$

In the above formula, χ varies among the vectors in $[0, 1]^{\Gamma}$ such that $\sum_{\sigma} \chi_{\sigma} = 1$.

If the collection of vectors $\{F_{\sigma}(x)\}_{\sigma \in \Gamma}$ are the vertices of a simplex for any $x \in \Omega$ then this holds also for the vectors $\{-F_{\sigma}(x)\}_{\sigma \in \Gamma}$ and consequently we have

$$j_m^+(x, \dot{x}) = \begin{cases} j(x, \chi^{-F}(\dot{x})) & \text{if } \dot{x} \in \mathcal{C}(\{-F_{\sigma}(x)\}_{\sigma \in \Gamma}), \\ +\infty & \text{otherwise.} \end{cases} \quad (6.22)$$

Trivially, $\mathcal{C}(\{-F_{\sigma}(x)\}_{\sigma \in \Gamma}) = -\mathcal{C}(\{F_{\sigma}(x)\}_{\sigma \in \Gamma})$ and $\chi^{-F}(\dot{x}) = \chi^F(-\dot{x})$.

7. FLUCTUATION THEORY

In this section we further investigate the fluctuations of the mechanical variables of our PDMPs, following ideas and results developed in [1, 2, 3, 4] for interacting particle systems and inspired by the Freidlin and Wentzell theory [14] for diffusion processes. As we will show, PDMPs are a natural source of examples where the *macroscopic fluctuation theory* developed in [1, 2, 3, 4] applies. A key identity in this theory is given by the Fluctuation–Dissipation (FD) relation (7.9), which in [2] is a direct consequence of the Markov property, while the mechanical evolution of our PDMPs is not Markov. Hence,

the FD relation cannot be taken for granted in our case. In Subsection 7.2 we will prove it for the class of exactly solvable PDMPs with stationary measure given by (5.1) as well for PDMPs on the 1d torus not satisfying (5.1). Before considering these cases, in Subsection 7.1 we reformulate the results of [1, 2, 3, 4], in the simpler context of processes with trajectories in $C([0, T], \Omega)$ and discuss consequences of the FD relation (7.9).

7.1. General framework. We consider a λ -parameterized family of stochastic Markov processes with trajectories in $C([0, T], \Omega)$, satisfying a sample path LD principle as the parameter λ diverges to $+\infty$. This means that, fixed $\{\hat{x}(t)\}_{t \in [0, T]} \in C([0, T], \Omega)$, it holds

$$\mathbb{P}_{x_0}^\lambda \left(\{x(t)\}_{t \in [0, T]} \approx \{\hat{x}(t)\}_{t \in [0, T]} \right) \sim e^{-\lambda I_{[0, T]}^{x_0}(\{\hat{x}(t)\}_{t \in [0, T]})}, \quad (7.1)$$

where in the above formula $\{x(t)\}_{t \in [0, T]}$ denotes a generic element of $C([0, T], \Omega)$ and $\mathbb{P}_{x_0}^\lambda$ denotes the law on $C([0, T], \Omega)$ induced by the λ -parameterized process with initial configuration $x_0 \in \Omega$. As a prototype one can take diffusions on $\Omega = \mathbb{R}^d$ with noise of order $\sqrt{1/\lambda}$ as in the Freidlin and Wentzell theory [14].

We further assume that for any fixed λ the λ -parameterized process admits a unique invariant measure ρ_λ . Then the adjoint process can be defined and has ρ_λ as unique invariant measure. We assume that also the λ -parameterized family of adjoint processes satisfies a LD principle as λ diverges, i.e. (7.1) remains valid with $\mathbb{P}_{x_0}^\lambda$ and $I_{[0, T]}^{x_0}$ replaced by $\mathbb{P}_{x_0}^{\lambda,+}$ and $I_{[0, T]}^{x_0,+}$, respectively. In addition, we assume that there exist densities $\mathcal{L}(x, \dot{x}), \mathcal{L}^+(x, \dot{x}) : \Omega \times \mathbb{R}^d \rightarrow [0, \infty)$ such that for any initial configuration x_0 the rate functionals $I_{[0, T]}^{x_0}$ and $I_{[0, T]}^{x_0,+}$ admit an integral representation of the form

$$I_{[0, T]}^{x_0}(\{x(t)\}_{t \in [0, T]}) = \begin{cases} \int_0^T \mathcal{L}(x(t), \dot{x}(t)) dt & \text{if } x(\cdot) \in \mathcal{X}_{x_0}, \\ +\infty & \text{otherwise,} \end{cases} \quad (7.2)$$

$$I_{[0, T]}^{x_0,+}(\{x(t)\}_{t \in [0, T]}) = \begin{cases} \int_0^T \mathcal{L}^+(x(t), \dot{x}(t)) dt & \text{if } x(\cdot) = \mathcal{X}_{x_0}^+, \\ +\infty & \text{otherwise,} \end{cases} \quad (7.3)$$

for suitable subspaces $\mathcal{X}_{x_0}, \mathcal{X}_{x_0}^+ \subset C([0, T], \Omega)$. This assumption implies in particular that all paths in \mathcal{X}_{x_0} and $\mathcal{X}_{x_0}^+$ starts in x_0 .

The functions \mathcal{L} and \mathcal{L}^+ are called Lagrangians. Typically, $\mathcal{L}(x, \dot{x}) = 0$ if and only if $\dot{x} = \bar{F}(x)$ for a suitable vector field $\bar{F}(x)$ that identifies the law of large numbers of the model in the limit of diverging λ . In fact, in this case, from (7.1) we can immediately derive that

$$\lim_{\lambda \rightarrow +\infty} \mathbb{P}_{x_0}^\lambda \left(\sup_{t \in [0, T]} |x(t) - \bar{x}(t)| > \delta \right) = 0, \quad \forall \delta > 0, \quad (7.4)$$

where $\{\bar{x}(t)\}_{t \in [0, T]} \in C([0, T], \Omega)$ solves the Cauchy problem

$$\begin{cases} \dot{\bar{x}}(t) = \bar{F}(\bar{x}(t)), \\ \bar{x}(0) = x_0. \end{cases} \quad (7.5)$$

Similarly we require that \mathcal{L}^+ vanishes along a path $\{x(t)\}_{t \in [0, T]}$ if and only if $\dot{x}(t) = \bar{F}^+(x(t))$, where the vector field \bar{F}^+ identifies the law of large numbers of the adjoint process in the limit of diverging λ .

Finally we assume that the family of invariant measures ρ_λ satisfy a LD principle on Ω as λ diverges, with rate function $V(x)$. This means that for any fixed t and for any fixed

$x \in \Omega$ it holds

$$\mathbb{P}_{\rho_\lambda}^\lambda (x(t) \approx x) \sim e^{-\lambda V(x)}, \quad (7.6)$$

where $\mathbb{P}_{\rho_\lambda}^\lambda$ denotes the law of the stationary process with parameter λ and initial distribution ρ_λ . Below we will denote by $\mathbb{P}_{\rho_\lambda}^{\lambda,+}$ the law of its adjoint process.

Let us now derive some consequences from our assumptions. By definition we have for any path $x(\cdot) \in C([-T, T], \Omega)$ that

$$\mathbb{P}_{\rho_\lambda}^\lambda \left(\{X(t)\}_{t \in [-T, T]} \approx \{x(t)\}_{t \in [-T, T]} \right) = \mathbb{P}_{\rho_\lambda}^{\lambda,+} \left(\{X(t)\}_{t \in [-T, T]} \approx \{x(-t)\}_{t \in [-T, T]} \right). \quad (7.7)$$

Due to the fact that the processes are Markov and that the path $\{x(t-T)\}_{t \in [0, 2T]}$ belongs to the path space $\mathcal{X}_{x(-T)}$ (referred to the time interval $[0, 2T]$), while the path $\{x(T-t)\}_{t \in [0, 2T]}$ belongs to the path space $\mathcal{X}_{x(T)}$ (referred to the time interval $[0, 2T]$), (7.7) implies the following relation concerning the LD rate functionals:

$$V(x(-T)) + \int_{-T}^T \mathcal{L}(x(t), \dot{x}(t)) dt = V(x(T)) + \int_{-T}^T \mathcal{L}^+(x(-t), -\dot{x}(-t)) dt. \quad (7.8)$$

Dividing both sides of (7.8) by $2T$ and taking the limit $T \downarrow 0$ we obtain FD relation

$$\mathcal{L}(x, \dot{x}) = \nabla V(x) \cdot \dot{x} + \mathcal{L}^+(x, -\dot{x}), \quad (7.9)$$

valid for any x, \dot{x} corresponding to the values $x(0), \dot{x}(0)$ for some path $x(\cdot)$ as above.

From now on we suppose that the FD relation (7.9) holds, without assuming that the processes under consideration are Markov. Following [2] we derive some consequences of (7.9).

A point $x_* \in \Omega$ is called *equilibrium point* for the λ -parameterized family of processes if $\bar{F}(x_*) = 0$. Then, by the LLN (7.4), the trajectory $\bar{x}(t) \equiv x_*$ is the limiting path for the process starting in x_* , thus implying that $I_{[0, T]}^{x_*}(\bar{x}(\cdot)) = 0$, i.e. $\mathcal{L}(x_*, 0) = 0$. By means of the FD relation we obtain that $\mathcal{L}^+(x_*, 0) = 0$ and consequently x_* is an equilibrium point also for the family of adjoint processes, i.e. we have $\bar{F}^+(x_*) = 0$. We restrict now to the case that the vector field \bar{F} has a unique equilibrium point x_* , which is a global attractor. This means that

$$\lim_{t \rightarrow +\infty} x(t) = x_*$$

for any $\{x(t)\}_{t \in [0, +\infty)}$ solving $\dot{x} = \bar{F}(x)$. Note that, due to the previous argument, x_* is also the unique equilibrium point of the vector field \bar{F}^+ . We assume that it is also a global attractor for \bar{F}^+ . As simple example satisfying all the above assumptions, consider the family of reversible diffusions on $\Omega = \mathbb{R}^d$ described by the SDE

$$\dot{x} = -\nabla U(x) + \lambda^{-\frac{1}{2}} \dot{w},$$

where U is a single well potential and w is a standard Brownian motion. In this case

$$\mathcal{L}(x, \dot{x}) = \mathcal{L}^+(x, \dot{x}) = \frac{1}{2} |\dot{x} + \nabla U(x)|^2,$$

and $V(x) = 2U(x)$.

Let us introduce the *quasi-potential* $Q(x)$ as function on Ω defined by

$$Q(x) = \inf_{\mathcal{A}_x} \int_{-\infty}^0 \mathcal{L}(x(t), \dot{x}(t)) dt, \quad (7.10)$$

where

$$\mathcal{A}_x = \left\{ \{x(t)\}_{t \in (-\infty, 0]} : x(0) = x, \lim_{t \rightarrow -\infty} x(t) = x_* \right\}.$$

In the case of multiple equilibrium points and different basins of attraction the definition has to be suitably modified. We will not consider this situation here, referring to [14] the interested reader.

Remark 1. *We point out that the rigorous definition of quasi-potential is slightly different from (7.10). Indeed, since the dynamic LD principles with rate functionals (7.2), (7.3) hold for finite time intervals, one has to define the quasi-potential as*

$$Q(x) = \inf_{T \geq 0} \inf_{\mathcal{A}_x^T} \int_{-T}^0 \mathcal{L}(x(t), \dot{x}(t)) dt, \quad (7.11)$$

where

$$\mathcal{A}_x^T = \left\{ \{x(t)\}_{t \in [-T, 0]} : x(0) = x, x(-T) = x_* \right\}.$$

We use definition (7.10) to simplify our discussion, while the interested reader can adapt our arguments in order to obtain rigorous proofs (see for example [5]).

We now derive an *H-Theorem* for the quasi-potential. More precisely, we show that the quasi-potential is a decreasing Lyapunov functional for both the vector field \bar{F} and for the vector field \bar{F}^+ . This means that $t \rightarrow Q(x(t))$ is a decreasing function if $\dot{x}(t) = \bar{F}(x(t))$ or if $\dot{x}(t) = \bar{F}^+(x(t))$, respectively. In order to justify our claim, we take a path $\{x(t)\}_{t \geq 0}$ such that $\dot{x}(t) = \bar{F}(x(t))$. Let $x = x(0)$ and $x' = x(t')$, with $t' > 0$. Given $\varepsilon > 0$ we fix an element $\{\tilde{x}(t)\}_{t \in [-\infty, 0]} \in \mathcal{A}_x$ such that $Q(x)$ differs from $I_{(-\infty, 0]}(\tilde{x}(\cdot))$ at most ε . Then we construct the following element of $\mathcal{A}_{x'}$

$$\bar{x}(t) = \begin{cases} \tilde{x}(t + t') & \text{if } t \leq -t', \\ x(t + t') & \text{if } t \in (-t', 0]. \end{cases}$$

Since $\mathcal{L}(x(t), \dot{x}(t)) = 0$ for all $t \geq 0$, we have

$$\begin{aligned} Q(x') &\leq \int_{-\infty}^0 \mathcal{L}(\bar{x}(t), \dot{\bar{x}}(t)) dt = \int_{-\infty}^{-t'} \mathcal{L}(\tilde{x}(t + t'), \dot{\tilde{x}}(t + t')) dt + \\ &\quad \int_{-t'}^0 \mathcal{L}(x(t + t'), \dot{x}(t + t')) dt = \int_{-\infty}^0 \mathcal{L}(\tilde{x}(t), \dot{\tilde{x}}(t)) dt \leq Q(x) + \varepsilon. \end{aligned}$$

By the arbitrariness of ε , we deduce that $Q(x') \leq Q(x)$. Therefore, it must be $\nabla Q(x) \cdot \bar{F}(x) \leq 0$ for all $x \in \Omega$. The same kind of argument can be used for the vector fields \bar{F}^+ , thus implying that $\nabla Q(x) \cdot \bar{F}^+(x) \leq 0$.

Let us now show that the quasi-potential $Q(x)$ coincides with the LD rate functional $V(x)$ of the invariant measures ρ_λ :

$$Q(x) = V(x) \quad \forall x \in \Omega.$$

Since \mathcal{L}^+ is nonnegative, using the FD relation we get for any $\{x(t)\}_{t \in [-\infty, 0]} \in \mathcal{A}_x$ that

$$\int_{-\infty}^0 \mathcal{L}(x(t), \dot{x}(t)) dt \geq \int_{-\infty}^0 \nabla V(x(t)) \cdot \dot{x}(t) dt = V(x) - V(x_*) = V(x). \quad (7.12)$$

The last equality follows from the fact that the rate functional V is zero on the unique equilibrium point x_* . The function V is in fact non negative due to the fact that it is a rate functional and it is zero in correspondence of x^* that corresponds to the typical

value (law of large numbers). Due to the definition of the quasi-potential Q , the above bound (7.12) implies that $Q(x) \geq V(x)$. In order to prove the reversed inequality, let $\{x^+(t)\}_{t \in [0, +\infty]}$ be the solution of the Chauchy problem

$$\begin{cases} \dot{x}^+(t) = \bar{F}^+(x^+(t)), \\ x^+(0) = x. \end{cases} \quad (7.13)$$

Due to the global attractiveness of x_* we have

$$\lim_{t \rightarrow +\infty} x^+(t) = x_*,$$

so that $\mathcal{T}[\{x^+(t)\}_{t \in [0, +\infty]}] = \{x^+(-t)\}_{t \in [-\infty, 0]} \in \mathcal{A}_x$ and, by definition of $Q(x)$ and due to the FD relation (7.9),

$$Q(x) \leq \int_{-\infty}^0 \mathcal{L}(x^+(-t), -\dot{x}^+(-t)) dt = V(x),$$

thus concluding the proof that $Q(x) = V(x)$. Coming back to the above expression, we then conclude that the path $\{x^+(-t)\}_{t \in [-\infty, 0]}$ is the minimizer in (7.10). Hence, we arrive at the following key observation. Starting from equilibrium at time zero, for λ and T large, if the system at time T is in state x then with high probability its evolution for times $t \in [0, T]$ is well approximated by the path $x^+(T - \cdot)$, where $x^+(\cdot)$ solves (7.13). More precisely:

$$\begin{aligned} \lim_{T \uparrow \infty} \lim_{\lambda \uparrow \infty} \mathbb{P}_{\rho_\lambda}^\lambda \left(\{x(t)\}_{t \in [0, T]} \approx \{x^+(T - t)\}_{t \in [0, T]} \middle| x(T) = x \right) = \\ \lim_{T \uparrow \infty} \lim_{\lambda \uparrow \infty} \mathbb{P}_{\rho_\lambda}^\lambda \left(\{x(t)\}_{t \in [-T, 0]} \approx \{x^+(-t)\}_{t \in [-T, 0]} \middle| x(0) = x \right) = 1. \end{aligned} \quad (7.14)$$

We call $\{x^+(-t)\}_{t \in [0, \infty]}$ the *exit trajectory*, while we call the path $\{\bar{x}(t)\}_{t \in [0, +\infty]}$ solving (7.5) the *relax trajectory* (motivated by the LLN). When the vector fields \bar{F} and \bar{F}^+ coincide, i.e.

$$\bar{F}(x) = \bar{F}^+(x), \quad \forall x \in \Omega, \quad (7.15)$$

then the exit/relax trajectories are related by time reversal and using the terminology of [1], [2] we say that an *Onsager-Machlup symmetry* holds. When condition (7.15) does not hold, the exit/relax trajectories are not necessarily related by time reversal and according to [1], [2] we say that a *generalized Onsager-Machlup symmetry* holds.

We conclude this subsection justifying the name ‘‘Lagrangian’’ given to $\mathcal{L}(x, \dot{x})$. From classical arguments in variational analysis it follows that the quasi-potential $Q(x)$ as defined in (7.10) solves the Hamilton-Jacobi equation

$$\mathcal{H}(x, \nabla Q(x)) = 0, \quad (7.16)$$

where the Hamiltonian \mathcal{H} is obtained as Legendre transform of \mathcal{L} as

$$\mathcal{H}(x, p) = \sup_{y \in \mathbb{R}^d} (p \cdot y - \mathcal{L}(x, y)). \quad (7.17)$$

It can be shown (see [2] for details) that Q is the maximal solution of (7.16). The r.h.s. of (7.16) must be zero for the following reason. Due to (7.17) it must be $\mathcal{H}(x_*, 0) = 0$, while due to the fact that $Q(x) \geq Q(x_*)$ it must be $\nabla Q(x_*) = 0$. Hence, $\mathcal{H}(x_*, \nabla Q(x_*)) = 0$.

Clearly the above arguments hold also for the family of adjoint processes. In particular, the quasi-potential Q solves also Hamilton-Jacobi equation

$$\mathcal{H}^+(x, \nabla Q(x)) = 0, \quad (7.18)$$

where the Hamiltonian \mathcal{H}^+ is obtained as Legendre transform of \mathcal{L}^+ as

$$\mathcal{H}^+(x, p) = \sup_{y \in \mathbb{R}^d} (p \cdot y - \mathcal{L}^+(x, y)) . \quad (7.19)$$

Note that due to the validity of the FD relation (7.9) we have

$$\begin{aligned} \mathcal{H}(x, p) &= \sup_{y \in \mathbb{R}^d} (p \cdot y - \mathcal{L}(x, y)) \\ &= \sup_{y \in \mathbb{R}^d} (p \cdot y - \nabla V(x) \cdot y - \mathcal{L}^+(x, -y)) \\ &= \sup_{y \in \mathbb{R}^d} ((\nabla V(x) - p) \cdot y - \mathcal{L}^+(x, y)) = \mathcal{H}^+(x, \nabla V(x) - p) . \end{aligned}$$

7.2. Application to PDMPs. In this subsection we further analyze the fluctuations of the process $x(t)$ describing the evolution of the mechanical state in our PDMPs, according to the results just described. As already stressed, the theory described in the previous subsection is based on the FD relation (7.9), which is always true if the process under consideration is Markov. In the case of PDMPs, the Markov property of $x(t)$ is typically violated. We check here the validity of the FD relation for a large class of PDMPs. That automatically implies the discussion following (7.9).

7.2.1. PDMPs with invariant measure of the form (5.1). Let us first restrict to PDMPs with invariant measure of the form (5.1), for which we can apply the results of Section 6 also to the adjoint process. The vector fields \bar{F} and \bar{F}^+ mentioned in the previous subsection become

$$\begin{cases} \bar{F}(x) = \sum_{\sigma} \mu(\sigma|x) F_{\sigma}(x) , \\ \bar{F}^+(x) = - \sum_{\sigma} \mu^+(\sigma|x) F_{\sigma}(x) . \end{cases}$$

We recall that $\mu(\cdot|x)$ and $\mu^+(\cdot|x)$ are the unique invariant measures of $L_c[x]$ and $L_c^+[x]$, respectively.

We already stressed that the mechanical process is in general not Markovian and consequently there is not a natural notion of invariant measure. This has to be replaced by the projection $\hat{\rho}_{\lambda}$ on the x component of the invariant measure of the joint mechanical and chemical Markov process

$$\hat{\rho}_{\lambda}(x) := \sum_{\sigma} \rho_{\lambda}(x, \sigma) .$$

In this case it is easy to compute the limit $\lim_{\lambda \rightarrow \infty} \lambda^{-1} \log \hat{\rho}_{\lambda}(x)$, and derive a LD principle for $\hat{\rho}$. To this aim, first observe that the function S in (5.1) is univocally determined up to an additive constant. From now on, we denote by S the unique function satisfying (5.1) normalized in such a way that $\inf_{x \in \Omega} S(x) = 0$. By this choice, it is simple to see that

$$\lim_{\lambda \rightarrow \infty} \lambda^{-1} \log \hat{\rho}_{\lambda}(x) = -S(x) .$$

Comparing with (7.6), we deduce that $S(x) = V(x)$, namely the function S coincides with the LD rate functional of the measures $\hat{\rho}_{\lambda}$.

We now establish for this class of models the symmetry relation

$$j(x, \chi) - j^+(x, \chi) = \sum_{\sigma} \chi_{\sigma} (\gamma(\sigma|x) - \gamma^+(\sigma|x)) , \quad (7.20)$$

for the joint rate density j and j^+ introduced in 6.

When $L_c[x]$ and consequently also $L_c^+[x]$ are reversible w.r.t. the corresponding quasi-stationary measures, then (7.20) follows directly from the explicit expressions (6.9) and (6.19). In the general case we can write the variational expressions (6.7) and (6.17) as

$$j(x, \chi) = \sum_{\sigma} \chi_{\sigma} \gamma(\sigma|x) - \inf_{z \in (0, +\infty)^{\Gamma}} \left(\sum_{(\sigma, \sigma') \in W} \chi_{\sigma} r(\sigma, \sigma'|x) \frac{z_{\sigma'}}{z_{\sigma}} \right), \quad (7.21)$$

$$j^+(x, \chi) = \sum_{\sigma} \chi_{\sigma} \gamma^+(\sigma|x) - \inf_{z \in (0, +\infty)^{\Gamma}} \left(\sum_{(\sigma, \sigma') \in W} \chi_{\sigma'} r(\sigma, \sigma'|x) \frac{\rho(x, \sigma) z_{\sigma}}{\rho(x, \sigma') z_{\sigma'}} \right). \quad (7.22)$$

When $\chi_{\sigma} > 0$ for any $\sigma \in \Gamma$ we introduce $\tilde{z}_{\sigma} := \frac{\chi_{\sigma}}{\rho(x, \sigma) z_{\sigma}}$. The variational expression in (7.22) can then be written as

$$\inf_{\tilde{z} \in (0, +\infty)^{\Gamma}} \left(\sum_{(\sigma, \sigma') \in W} \chi_{\sigma} r(\sigma, \sigma'|x) \frac{\tilde{z}_{\sigma'}}{\tilde{z}_{\sigma}} \right),$$

that coincides with the variational expression in (7.21). Relation (7.20) now follows immediately. The same result can be obtained also in the case that there exists some $\sigma \in \Gamma$ for which $\chi_{\sigma} = 0$. We discuss this case in Appendix D.

Using equations (5.9) (valid for each $\sigma \in \Gamma$), which are equivalent to the second group of equations in (5.7), we obtain that (7.20) can be written as

$$j(x, \chi) - j^+(x, \chi) = \nabla S(x) \cdot \left(\sum_{\sigma} \chi_{\sigma} F_{\sigma} \right). \quad (7.23)$$

Observe that to compute both $j_m(x, \dot{x})$ and $j_m^+(x, -\dot{x})$ we need to minimize respectively j and j^+ over χ subject to the same constraint

$$\left\{ \sum_s \chi_s F_{\sigma}(x) = \dot{x} \right\}. \quad (7.24)$$

Recalling (7.23), we get for any fixed x and \dot{x} that

$$\begin{aligned} j_m(x, \dot{x}) &= \inf_{\{\chi: \sum_s \chi_s F_{\sigma}(x) = \dot{x}\}} j(x, \chi) \\ &= \nabla S(x) \cdot \dot{x} + \inf_{\{\chi: \sum_s \chi_s F_{\sigma}(x) = \dot{x}\}} j^+(x, \chi) \\ &= \nabla S(x) \cdot \dot{x} + j_m^+(x, -\dot{x}). \end{aligned} \quad (7.25)$$

That corresponds to the FD relation (7.9) since, as already observed, $S(x) = V(x)$. From (7.25) we obtain also that the minimizers in (7.24) for the computation of both $j_m(x, \dot{x})$ and $j_m^+(x, -\dot{x})$, coincide. We point out that in the case of computable LD rate functionals as in (6.14) and (6.22), identity (7.25) follows directly from (6.9), (6.19) and the simple relation $\chi_{\sigma}^F(\dot{x}) = \chi_{\sigma}^{-F}(-\dot{x})$.

It is interesting to note that we can obtain a simple explicit expression for the *entropy production*, i.e. the rate of variation of S along the orbits of the vector fields \bar{F} and \bar{F}^+ . Given $x(t)$ a solution of (7.5), using (5.9) we have

$$\nabla S(x) \cdot \dot{x} = \nabla S(x) \cdot \bar{F}(x) = \sum_{\sigma} \mu(\sigma|x) \nabla S(x) \cdot F_{\sigma}(x) = \sum_{\sigma} \mu(\sigma|\bar{x}) (\gamma(\sigma|x) - \gamma^+(\sigma|x)). \quad (7.26)$$

Likewise given x^+ a solution of (7.13) we have

$$\nabla S(x^+) \cdot \dot{x}^+ = \sum_{\sigma} \mu^+(\sigma|x^+) (\gamma^+(\sigma|x^+) - \gamma(\sigma|x^+)) . \quad (7.27)$$

We now illustrate with examples the validity of the general results discussed in subsection 7.1 for PDMPs. We stress that these results are a direct consequence of the FD relation (7.9) checked above. We first consider the 1D models of Subsection 4.1. In this case the quasistationary measures for the direct and adjoint chemical generators can be easily computed and we have

$$\begin{cases} \bar{F}(x) = \frac{r(1,0|x)}{r(1,0|x)+r(0,1|x)} F_0(x) + \frac{r(0,1|x)}{r(1,0|x)+r(0,1|x)} F_1(x), \\ \bar{F}^+(x) = - \left(\frac{r(1,0|x)F_0^2(x)}{r(1,0|x)F_0^2(x)+r(0,1|x)F_1^2(x)} F_1(x) + \frac{r(0,1|x)F_1^2(x)}{r(1,0|x)F_0^2(x)+r(0,1|x)F_1^2(x)} F_0(x) \right). \end{cases} \quad (7.28)$$

Note that $x \in \Omega$ is an equilibrium point for \bar{F} if and only if

$$r(1,0|x)F_0(x) + r(0,1|x)F_1(x) = 0.$$

The same equation characterizes the equilibrium points of \bar{F}^+ , thus implying that \bar{F} and \bar{F}^+ have the same equilibrium points in Ω . Moreover we have that both relations $\bar{F}(x) > 0$ and $\bar{F}^+(x) > 0$ holds if and only if

$$r(1,0|x)F_0(x) + r(0,1|x)F_1(x) > 0,$$

so that also the stability of the equilibrium points for both vector fields is the same. We point out that, since $F_0(a) = F_1(b) = 0$, the adjoint vector field \bar{F}^+ has two additional equilibrium points at the boundary $\partial\Omega = \{a, b\}$, which are necessary unstable.

Note that there are models such that the vector field \bar{F} has many stable equilibrium points. In this case the definition of the quasi-potential $Q(x)$ in (7.10) has to be modified considering separately the different basin of attraction. We do not discuss this possibility.

For a vector $\dot{x} \in \mathcal{C}\{F_0(x), F_1(x)\}$ we have that

$$\chi_0^F(\dot{x}) = \frac{F_1(x) - \dot{x}}{F_1(x) - F_0(x)}, \quad \chi_1^F(\dot{x}) = \frac{\dot{x} - F_0(x)}{F_1(x) - F_0(x)}.$$

Using the results of section 6 (see (6.10) and (6.14)), we get

$$j_m(x, \dot{x}) = \left(\sqrt{\frac{r(0,1|x)(F_1(x) - \dot{x})}{F_1(x) - F_0(x)}} - \sqrt{\frac{r(1,0|x)(\dot{x} - F_0(x))}{F_1(x) - F_0(x)}} \right)^2 \quad (7.29)$$

for all $x \in \Omega$ and $\dot{x} \in \mathcal{C}(F_0(x), F_1(x))$. Since similarly to (6.10)+(6.14) it holds

$$j_m^+(x, \dot{x}) = \left(\sqrt{\chi_0^{-F}(\dot{x})r^+(0,1|x)} - \sqrt{\chi_1^{-F}(\dot{x})r^+(1,0|x)} \right)^2, \quad (7.30)$$

observing that $\chi^{-F}(\dot{x}) = \chi^F(-\dot{x})$ for all $\dot{x} \in \mathcal{C}(-F_0(x), -F_1(x))$ we conclude that

$$j_m^+(x, \dot{x}) = \left(\sqrt{\frac{r(1,0|x)|F_0(x)|(F_1(x) + \dot{x})}{F_1(x)(F_1(x) - F_0(x))}} - \sqrt{\frac{r(0,1|x)F_1(x)(-\dot{x} - F_0(x))}{|F_0(x)|(F_1(x) - F_0(x))}} \right)^2 \quad (7.31)$$

for all $x \in \Omega$ and $\dot{x} \in \mathcal{C}(-F_0(x), -F_1(x))$. The validity of the FD relation (7.9) can now be checked directly recalling that in this case

$$\nabla S(x) = \frac{r(0,1|x)}{F_0(x)} + \frac{r(1,0|x)}{F_1(x)}. \quad (7.32)$$

Also the validity of the H-Theorem can be checked directly, we have in fact

$$\nabla S(x) \cdot \bar{F}(x) = -\frac{\left(r(1, 0|x)\sqrt{\frac{|F_0(x)|}{F_1(x)}} + r(0, 1|x)\sqrt{\frac{|F_1(x)|}{|F_0(x)|}}\right)^2}{r(0, 1|x) + r(1, 0|x)},$$

and

$$\nabla S(x) \cdot \bar{F}^+(x) = -\frac{\left(r(0, 1|x)F_1(x) + r(1, 0|x)F_0(x)\right)^2}{r(0, 1|x)F_1^2(x) + r(1, 0|x)F_0^2(x)},$$

whose negativity is immediate. Finally we can also explicitly compute the Hamiltonian

$$\mathcal{H}(x, p) = \sup_{y \in \mathcal{C}\{F_0(x), F_1(x)\}} [py - j_m(x, y)],$$

and check that (7.32) is its maximal solution. The solution to this variational problem is given by

$$\mathcal{H}(x, p) = p\dot{x}(x, p) - j_m(x, \dot{x}(x, p)),$$

where

$$\dot{x}(x, p) = \frac{1}{2}(F_1(x) + F_0(x)) + \frac{1}{2}(F_1(x) - F_0(x))\sqrt{\frac{\varepsilon(x, p)}{(\varepsilon(x, p) + 4)}}$$

and

$$\varepsilon(x, p) = \left((F_1(x) - F_0(x)) \frac{p}{\sqrt{r(0, 1|x)r(1, 0|x)}} + \frac{r(0, 1|x) - r(1, 0|x)}{\sqrt{r(1, 0|x)r(0, 1|x)}} \right)^2.$$

It can be checked that the Hamilton-Jacobi equation $\mathcal{H}(x, \nabla S) = 0$ holds. We refer the reader to [19] for these computations and for more details on the one dimensional models on a bounded domain.

In the case of the triangular domain with unitary jump rates discussed in subsection 5.2 we have

$$\bar{F}(x, y) = \left(\frac{1}{3} - x, \frac{1}{3} - y \right)$$

and

$$\bar{F}^+(x, y) = \left(x - \frac{x^2}{x^2 + y^2 + (1 - x - y)^2}, y - \frac{y^2}{x^2 + y^2 + (1 - x - y)^2} \right). \quad (7.33)$$

The vector field \bar{F} has an unique stable equilibrium point $(\frac{1}{3}, \frac{1}{3}) \in \Omega$, which is globally attractive. The vector field \bar{F}^+ has $(\frac{1}{3}, \frac{1}{3})$ as unique stable equilibrium point in Ω , which is globally attractive for all other points of Ω . Moreover \bar{F}^+ has also unstable equilibrium points belonging to $\partial\Omega$. These are given by $(0, 0)$, $(0, \frac{1}{2})$, $(0, 1)$, $(\frac{1}{2}, 0)$, $(1, 0)$ and $(\frac{1}{2}, \frac{1}{2})$.

The validity of the H-Theorem can be checked directly recalling the expression (5.40) and computing

$$\nabla S(x, y) \cdot \bar{F}(x, y) = \frac{1}{3} \left(9 - \frac{1}{x} - \frac{1}{y} - \frac{1}{1 - x - y} \right).$$

The above expression is negative due to the fact $\frac{1}{x} + \frac{1}{y} + \frac{1}{z} \geq 9$ when x, y and z are constrained to satisfy the relation $x + y + z = 1$ (this follows from the convexity of

$x \rightarrow 1/x$). We can also compute

$$\nabla S(x, y) \cdot \bar{F}^+(x, y) = \frac{1}{x^2 + y^2 + (1 - x - y)^2} - 3$$

that is negative due to the fact that $\frac{1}{x^2 + y^2 + z^2} \leq 3$ when x, y and z are constrained to satisfy the relation $x + y + z = 1$ (again by convexity).

Finally, we point out that our general considerations allow to solve non trivial variational problems. Consider for example the problem to determine the infimum

$$\inf_{\mathcal{A}(x, y)} \int_{-\infty}^0 \left(2 - \sum_{(\sigma, \sigma') \in W} \sqrt{\chi_\sigma(t)} \sqrt{\chi_{\sigma'}(t)} \right) dt, \quad (7.34)$$

where $\mathcal{A}(x, y)$ denotes the family of continuous paths $z(t) : (-\infty, 0] \rightarrow \mathbb{R}^2$, such that (i) $\lim_{t \downarrow -\infty} z(t) = (1/3, 1/3)$, (ii) $z(0) = (x, y)$, (iii) $\dot{z}(t)$ belongs to the convex hull $C\{F_1(z(t)), F_2(z(t)), F_3(z(t))\}$, while $(\chi_1(t), \chi_2(t), \chi_3(t))$ denotes the unique probability measure such that $\dot{z}(t) = \sum_{\sigma=1}^3 \chi_\sigma(t) F_\sigma(z(t))$. This last identity is equivalent to the system

$$\begin{cases} \chi_1(t) = 1 - x(t) - y(t) - \dot{x}(t) - \dot{y}(t), \\ \chi_2(t) = x(t) + \dot{x}(t), \\ \chi_3(t) = y(t) + \dot{y}(t). \end{cases}$$

Since the integrand in (7.34) is the LD functional density $j(x(t), \chi(t))$ (cf. (6.9)), while $(1/3, 1/3)$ is the equilibrium point of the vector field \bar{F} , we know that the minimal value in (7.34) is given by the quantity $S(x, y)$ in (5.40), after suitable renormalization. More precisely, the solution of (7.34) equals

$$-\log x - \log y - \log(1 - x - y) - 3 \log 3.$$

Moreover, the minimizer in (7.34) is obtained by time-inversion of the solution of the Chauchy problem

$$\begin{cases} (\dot{x}(t), \dot{y}(t)) = \bar{F}^+(x(t), y(t)), \\ (x(0), y(0)) = (x, y), \end{cases}$$

where the vector field \bar{F}^+ is computed in (7.33).

7.2.2. Generalizations of identity (7.25). As already observed, the validity of the FD relation for PDMPs with invariant measures of the form (5.1) follows from the identity (7.25). This key identity can be rewritten as

$$j_m(x, \dot{x}) = \nabla W \cdot \dot{x} + \mathcal{G}(x, -\dot{x}), \quad (7.35)$$

where $W = S$ and $\mathcal{G}(x, -\dot{x}) = j_m^+(x, -\dot{x})$. In this subsection, we desire to present a conjecture related to (7.35). In general, the computation of the quasi-potential (7.10) for PDMPs not having invariant measure of the form (5.1) is non trivial. We will discuss a specific example of this type in the next subsection. A possible purely variational approach to this problem is as follows. Suppose we can decompose the dynamic LD rate density as in (7.35), where now $\mathcal{G}(x, \dot{x})$ is a nonnegative function, which is zero only when $\dot{x} = G(x)$, with G a vector field having x_* as the unique global attractive equilibrium point. Then from the general arguments in subsection 7.1 we have that W coincides in fact with the quasi-potential Q . Inspired by the structure of the rate functionals for PDMPs we can search for \mathcal{G} having a specific form. For simplicity we discuss only the case of computable rates of the form (6.14) when the chemical part of the generator is reversible for any x

and consequently j is given by (6.9). In this case given a positive $\psi(\sigma, x)$ we can search for a \mathcal{G} of the form

$$\mathcal{G}(x, \dot{x}) = \sum_{\sigma} \tilde{\gamma}(\sigma|x) \chi_{\sigma}^{-F}(\dot{x}) - \sum_{(\sigma, \sigma') \in W} \sqrt{\frac{\mu(\sigma|x)}{\mu(\sigma'|x)}} r(\sigma, \sigma'|x) \sqrt{\chi_{\sigma}^{-F}(\dot{x})} \sqrt{\chi_{\sigma'}^{-F}(\dot{x})},$$

where

$$\tilde{\gamma}(\sigma|x) := \sum_{\sigma'} r(\sigma', \sigma|x) \frac{\psi(\sigma', x)}{\psi(\sigma, x)}.$$

To verify (7.35) we need to find a function W such that for any x, \dot{x} it holds

$$\sum_{\sigma} (\gamma(\sigma|x) - \tilde{\gamma}(\sigma|x)) \chi_{\sigma}^F(\dot{x}) = \nabla W \cdot \dot{x} = \sum_{\sigma} (\nabla W \cdot F_{\sigma}(x)) \chi_{\sigma}^F(\dot{x}). \quad (7.36)$$

To derive the above condition we used $\chi_{\sigma}^F(\dot{x}) = \chi_{\sigma}^{-F}(-\dot{x})$. Condition (7.36) is verified if and only if for any $\sigma \in \Gamma$ and for any $x \in \Omega$ we have that $\gamma(\sigma|x) - \tilde{\gamma}(\sigma|x)$ is the directional derivative of W at x along the direction $F_{\sigma}(x)$. In this case the vector field G is given by

$$G(x) = -\frac{1}{Z(x)} \sum_{\sigma} \frac{\psi^2(\sigma, x)}{\mu(\sigma|x)} F_{\sigma}(x),$$

where $Z(x) := \sum_{\sigma} \frac{\psi^2(\sigma, x)}{\mu(\sigma|x)}$. If we can find the positive functions ψ in such a way that the above requirements are satisfied then the function W obtained in (7.36), appropriately normalized, coincides with the quasi-potential. In this case we obtain also that \bar{F}^+ in fact coincides with G . We do not discuss this issue here.

7.2.3. PDMPs on the 1D torus. We now consider the PDMPs with $\Omega = \mathbb{R}/\mathbb{Z}$ discussed in Section 4.2. If the equilibrium condition (4.9) holds, then we know that the invariant measure has the form (5.1) and therefore the validity of relation (7.9) follows from the above discussion. We consider here the general case, without assuming (4.9).

Starting from the exact expression (4.6) of the invariant measure we can derive the LD functional of $\hat{\rho}_{\lambda}$. We have that

$$\lim_{\lambda \rightarrow \infty} \hat{\rho}_{\lambda}(x) = \lim_{\lambda \rightarrow \infty} \lambda^{-1} \log \left(\rho_{\lambda}(x, 0) + \rho_{\lambda}(x, 1) \right) = \sup_{y \in [x, x+1]} \left(S(y) - S(x) \right) + c =: -W(x), \quad (7.37)$$

where c is an appropriate additive constant related to the normalization factor $k = k(\lambda)$ in (4.6). Formula (7.37) follows from the fact that for arbitrary $a(\lambda)$ and $b(\lambda)$ it holds

$$\lim_{\lambda \rightarrow +\infty} \lambda^{-1} \log(a(\lambda) + b(\lambda)) = \max \left\{ \lim_{\lambda \rightarrow +\infty} \lambda^{-1} \log a(\lambda), \lim_{\lambda \rightarrow +\infty} \lambda^{-1} \log b(\lambda) \right\},$$

and from the Laplace theorem [11]. Note that the function W defined in (7.37), due to the validity of (4.7), satisfy the periodicity condition $W(x) = W(x+1)$ and consequently it can be interpreted as a function on the torus $\Omega = \mathbb{R}/\mathbb{Z}$. The constant c appearing in (7.37) can be computed observing that, since $\int_{\Omega} \hat{\rho}_{\lambda}(x) dx = 1$, the Laplace theorem implies that $\inf_{x \in [0, 1]} W(x) = 0$. Therefore, it must be

$$c = - \sup_{x \in [0, 1]} \sup_{y \in [x, x+1]} \left(S(y) - S(x) \right).$$

The above function W is the LD functional for the measure $\hat{\rho}_\lambda$. If the function S is periodic, then it is simple to check that $W(x) = S(x) - \min_{y \in [0,1]} S(y)$. In the general case, W is a nonnegative function that can be flat on subregions of Ω .

Let us now verify the validity of the FD relation (7.9), with $\mathcal{L}(x, \dot{x}) = j_m(x, \dot{x})$, $\mathcal{L}^+(x, \dot{x}) = j_m^+(x, \dot{x})$ and $V = W$. For simplicity, we assume the same conditions discussed after (4.13). The function $y(x)$ is defined as in the paragraph below (4.13). First we need to compute ∇W . We have that in the points where W is differentiable it holds

$$\nabla W(x) = \nabla S(x) - \nabla S(y(x)) \nabla y(x). \quad (7.38)$$

When $y(x) \in (x, x+1)$ we have that (7.38) becomes

$$\nabla W(x) = \nabla S(x), \quad (7.39)$$

due to the fact that $\nabla S(y(x)) = 0$. When $y(x) \in \{x, x+1\}$ then (7.38) becomes

$$\nabla W(x) = 0, \quad (7.40)$$

due to the fact that $\nabla S(x) = \nabla S(x+1)$ and $\nabla y(x) = 1$. Note that this second alternative holds for any x if the vector fields F_0 and F_1 have the same sign so that in this case W is identically zero.

The lagrangian $j_m(x, \dot{x})$ can be computed by means of (6.10) and (6.14), getting that its expression coincides with (7.29). The lagrangian $j_m^+(x, \dot{x})$ can be computed by adapting the arguments in [12]. We get that its expression can be obtained from (7.30) where instead of the λ -dependent rates r^+ we have to use their asymptotic limit value given by (4.14). We obtain for all $x \in \Omega$ and $\dot{x} \in \mathcal{C}(-F_0(x), -F_1(x))$

$$j_m^+(x, \dot{x}) = \left(\sqrt{\frac{r(1,0|x)B(x)(F_1(x) + \dot{x})}{F_1(x) - F_0(x)}} - \sqrt{\frac{r(0,1|x)(\dot{x} + F_0(x))}{B(x)(F_0(x) - F_1(x))}} \right)^2, \quad (7.41)$$

where $B(x) := \frac{F_0(x)}{F_1(x)} \frac{r(0,1|y(x))F_1(y(x))}{r(1,0|y(x))F_0(y(x))}$.

We can now compute $j_m(x, \dot{x}) - j_m^+(x, -\dot{x})$ obtaining

$$\begin{aligned} & \dot{x} \frac{\left[r(1,0|x) \left(1 + B(x) \right) - r(0,1|x) \left(1 + B^{-1}(x) \right) \right]}{F_1(x) - F_0(x)} + \\ & \frac{r(0,1|x) \left(F_1(x) + F_0(x) B^{-1}(x) \right) - r(1,0|x) \left(F_0(x) + F_1(x) B(x) \right)}{F_1(x) - F_0(x)}. \end{aligned} \quad (7.42)$$

The validity of the FD relation for points x where W is differentiable follows now directly from the fact that if $y(x) \in \{x, x+1\}$ then $B(x) = \frac{r(0,1|x)}{r(1,0|x)}$, while if $y(x) \in (x, x+1)$ then $B(x) = -\frac{F_0(x)}{F_1(x)}$ (recall 4.16). In particular the second term in (7.42) is identically zero.

Finally we point out that in the general case the quasi-potential cannot be defined directly as in (7.10). Indeed, the hypothesis of existence, uniqueness and global attractiveness of the equilibrium point of \bar{F} could be violated. We cannot then identify directly W with the quasi-potential.

8. A GALLAVOTTI-COHEN-TYPE SYMMETRY

In this section we briefly discuss a Gallavotti-Cohen-type (G-C) symmetry for PDMPs. Let us briefly recall a result of [17]. Consider an involution \mathcal{R} on the path space of a stochastic process, i.e. a map from the path space into itself such that $\mathcal{R}^2 = \mathbb{I}$. Assume

also that the measure $\mathbb{P}_{st} \circ \mathcal{R}^{-1}$ is absolutely continuous w.r.t. \mathbb{P}_{st} , where \mathbb{P}_{st} denotes the stationary measure of the process. Then the random variable

$$W_T := -\frac{1}{2T} \log \frac{d(\mathbb{P}_{st} \circ \mathcal{R}^{-1})}{d\mathbb{P}_{st}} \Big|_{t \in [-T, T]} \quad (8.1)$$

satisfies the G-C-type symmetry

$$\mathbb{E}_{st}(e^{-sW_T}) = \mathbb{E}_{st}(e^{-(1-s)W_T}), \quad (8.2)$$

where \mathbb{E}_{st} denotes the expectation w.r.t. \mathbb{P}_{st} .

Differently from the examples discussed in [17], for PDMPs it is natural to consider involutions \mathcal{R} different from time reversal. Indeed, take a trajectory $\{x(t), \sigma(t)\}_{t \in [-T, T]}$ of the PDMP, i.e. an element of $C([-T, T], \Omega) \times D([-T, T], \Gamma)$ such that for any continuity point $t \in [-T, T]$ of $\{\sigma(t)\}_{t \in [-T, T]}$ it holds

$$\dot{x}(t) = F_{\sigma(t)}(x(t)). \quad (8.3)$$

Then, the time reversed trajectory $\mathcal{T}[\{x(t), \sigma(t)\}_{t \in [-T, T]}] = \{x(-t), \sigma(-t)\}_{t \in [-T, T]}$ is typically not a trajectory of the PDMP due to the fact that if the vector fields F_σ are not identically zero then condition (8.3) is violated. In the case of PDMPs the absolutely continuous condition is equivalent to the preservation of relation (8.3). This means that for any trajectory $\{x(t), \sigma(t)\}_{t \in [-T, T]}$ also $\mathcal{R}[\{x(t), \sigma(t)\}_{t \in [-T, T]}]$ has to satisfy condition (8.3). We need then to find an involution \mathcal{R} on the path space preserving relation (8.3).

This is easily done for the following class of models. Consider a PDMP such that for any $\sigma \in \Gamma$ and for any $x \in \Omega$ there exists a unique $\sigma' \in \Gamma$ such that $F_{\sigma'}(x) = -F_\sigma(x)$. We call R_x the involution on Γ that associates to every σ the corresponding σ' characterized as above. Then the map \mathcal{R} defined as

$$\mathcal{R}[\{x(t), \sigma(t)\}_{t \in [-T, T]}] := \{x(-t), R_{x(-t)}\sigma(-t)\}_{t \in [-T, T]} \quad (8.4)$$

is an involution on the path space preserving (8.3). An example of such a PDMP is given by $\Omega = \mathbb{R}^2/\mathbb{Z}^2$, $\Gamma = \{1, 2, 3, 4\}$ and vector fields $F_i = e_i$, where e_1 and e_2 constitute the canonical basis of \mathbb{R}^2 and $e_3 = -e_1$, $e_4 = -e_2$. Then $R_x 1 = 3$, $R_x 2 = 4$, $R_x 3 = 1$ and $R_x 4 = 2$.

If we consider models satisfying additional assumptions we obtain an explicit form of the functional (8.1) having a direct physical interpretation. More precisely, we assume that the jump rates satisfy the generalized detailed balance condition

$$r(\sigma, \sigma'|x) = \exp\{H(\sigma, x) - H(\sigma', x)\} r(R_x \sigma', R_x \sigma|x), \quad (8.5)$$

for a suitable energy function $H : \Gamma \times \Omega \rightarrow \mathbb{R}$, and that the function $\gamma(\cdot|\cdot)$ satisfies

$$\gamma(\sigma|x) = \gamma(R_x \sigma|x), \quad \forall (x, \sigma) \in \Omega \times \Gamma. \quad (8.6)$$

This happens for example if we define the rates as

$$r(\sigma, \sigma'|x) := \exp\{[H(\sigma, x) - H(\sigma', x)]/2\}, \quad (8.7)$$

for an energy function H satisfying the symmetry condition

$$H(\sigma, x) = H(R_x \sigma, x), \quad \forall (x, \sigma) \in \Omega \times \Gamma. \quad (8.8)$$

Assuming (8.5) and (8.6), it is easy to compute (8.1) using standard methods for jump processes (see for example [15]). One gets up to boundary terms

$$W_T = \frac{1}{2T} \sum_i \{H(\sigma(\tau_i^-), x(\tau_i)) - H(\sigma(\tau_i), x(\tau_i))\}. \quad (8.9)$$

The boundary terms are due to the fact that in (8.1) we are considering stationary measures. In the case of compact phase space $\Omega \times \Gamma$ they are negligible in the limit of diverging T . In the above formula (8.9) the sum is over the jump times τ_i of $\{\sigma(t)\}_{t \in [-T, T]}$ and we denote the left limit as $\sigma(t^-) := \lim_{\Delta \downarrow 0} \sigma(t - \Delta)$. Since for any trajectory it holds

$$\begin{aligned} H(\sigma(T), x(T)) - H(\sigma(-T), x(-T)) &= \int_{-T}^T \nabla H(\sigma(s), x(s)) \cdot \dot{x}(s) ds \\ &\quad + \sum_i \{H(\sigma(\tau_i), x(\tau_i)) - H(\sigma(\tau_i^-), x(\tau_i))\}, \end{aligned}$$

in the case of bounded energy functions H we can derive from (8.9) that

$$W_T = \frac{1}{2T} \int_{-T}^T \nabla H(\sigma(s), x(s)) \cdot \dot{x}(s) ds + o(1), \quad (8.10)$$

which is the *averaged mechanical work done on the system by the external force fields* ∇H , apart negligible errors as $T \uparrow \infty$. Trivially, for PDMPs, (8.10) coincides with

$$W_T = \frac{1}{2T} \int_{-T}^T \nabla H(\sigma(s), x(s)) \cdot F_{\sigma(s)}(x(s)) ds + o(1). \quad (8.11)$$

APPENDIX A. EXTENDED GENERATOR

We first recall the definition of the Markov generator of the PDMP. A bounded measurable function $f : \Omega \times \Gamma \rightarrow \mathbb{R}$ is said to belong to the domain $\mathcal{D}(L)$ of L if the functions

$$\Omega \times \Gamma \ni (x, \sigma) \rightarrow t^{-1} \left[\mathbb{E}_{x, \sigma}^\lambda (f(x_t, \sigma_t)) - f(x, \sigma) \right] \quad (A.1)$$

converge uniformly (i.e. w.r.t. the uniform norm $\|\cdot\|_\infty$) to a bounded measurable function g as $t \downarrow 0$. In this case, one sets $Lf := g$.

As discussed in [10], if the jump rates $r(\sigma, \sigma'|x)$ are not uniformly bounded, it is a difficult task to characterize exactly the domain $\mathcal{D}(L)$ of the generator L . Moreover, $\mathcal{D}(L)$ could not contain very regular functions. Let us stress this last point by means of a simple example discussed in more detailed in Appendix B. We take $\Omega = (0, 1)$, $\Gamma = \{0, 1\}$, $F_0(x) = -1$, $F_1(x) = 1$, $r(0, 1|x) = 1/x$, $r(1, 0|x) = 1/(1-x)$. The associated PDMP satisfies all our assumptions. Indeed, $L_c[x]$ has a unique invariant measure, the number of jumps in a finite interval is finite a.s. due to (2.11) (see Appendix B), while the mechanical confinement in Ω is implied by (2.14). As discussed in Appendix B, the very regular function $f(x, \sigma) = \sigma$ does not belong to the domain $\mathcal{D}(L)$.

On the other hand, by standard computations, it is simple to prove that if the rates are bounded (as in the case that Ω is the d -dimensional torus), then functions $f(x, \sigma)$ which are bounded and C^1 in x belong to the domain $\mathcal{D}(L)$ of the generator and Lf equals (2.7). For general rates, the same computations allow to get the same conclusions for functions $f(x, \sigma)$ that are bounded, C^1 in x and with compact support inside Ω . In order to have a unified treatment, it is convenient to work with a weaker definition of generator L introduced by Davis (see [9], [10]), which allows a simple characterization of the domain $\mathcal{D}(L)$ and is strong enough to develop stochastic calculus for PDMPs. From now on, L

will denote the *extended generator*, whose domain $\mathcal{D}(L)$ is given by the set of measurable functions $f : \Omega \times \Gamma \rightarrow \mathbb{R}$ with the following property: there exists a measurable function $h : \Omega \times \Gamma \rightarrow \mathbb{R}$ such that the function $t \rightarrow h(x(t), \sigma(t))$ is integrable $\mathbb{P}_{x,\sigma}^\lambda$ -a.s. for all $(x, \sigma) \in \Omega \times \Gamma$ and the process

$$C_t^f := f(x(t), \sigma(t)) - f(x(0), \sigma(0)) - \int_0^t h(x(s), \sigma(s)) ds$$

is a local martingale. Then, one sets $Lf := h$. We have recalled here the definition of the extended generator for completeness, the reader non familiar with local martingales can skip it. We only use some consequences of the definition. In particular, we recall that L is an extension of the classical Markov generator, the domain $\mathcal{D}(L)$ of the extended generator admits a simple characterization and it includes all bounded functions $f(x, \sigma)$ which are C^1 in x (see Theorem (26.14) and Remark (26.16) in [10]). Moreover, for all functions f in $\mathcal{D}(L)$, Lf is given by (2.7). We point out that the theory in [10] is developed under the assumption that for any starting point (x, σ) the number N_t of jumps in the interval $[0, t]$ has finite expectation. As already observed, this condition is implied for example by (2.10).

APPENDIX B. AN EXAMPLE OF 1D PDMP WITH SINGULAR FEATURES

We consider the 1D PDMP such that $\Omega = (0, 1)$, $\Gamma = \{0, 1\}$, $F_0(x) = -1$, $F_1(x) = 1$, $r(0, 1|x) = 1/x$, $r(1, 0|x) = 1/(1-x)$. This PDMP satisfies all our assumptions. Indeed, $L_c[x]$ has a unique invariant measure $\mu(\cdot|x)$ given by (2.9), while the mechanical confinement in Ω is implied by (2.14). Moreover, we claim that the number of jumps in a finite interval is finite a.s. due to (2.11) (note that (2.10) is violated). To this aim suppose by contradiction that the family of jump times τ_k is a sequence converging to some $\tau_* < \infty$. Before time τ_* the mechanical state must be eventually in $(0, 3/4]$ or in $[1/4, 1)$ (otherwise it should evolve with arbitrarily large velocity). Let us consider for example the first case. Then, the system must be infinite times in the chemical state $\sigma = 1$ and, once it jumps into $\sigma = 1$, it remains in this chemical state for a random time typically of order one. This is in contradiction with the fact that $\tau_{k+1} - \tau_k$ converges to zero.

Let us now take $\lambda = 1$ and show another special feature of our simple PDMP: the regular function $f(x, \sigma) = \sigma$ does not belong to the domain of the classical (i.e. not extended) Markov generator. To this aim, let us start in the point $(x_0, 0)$. Then, the r.h.s. of (A.1) is simply $t^{-1}\mathbb{P}_{x_0,0}^1(\sigma_t = 1)$. If (A.1) has to converge uniformly to a bounded function as $t \downarrow 0$, then it must be

$$\limsup_{t \downarrow 0} \sup_{x_0 \in (0,1)} t^{-1}\mathbb{P}_{x_0,0}^1(\sigma_t = 1) < \infty. \quad (\text{B.1})$$

It is simple to check that the above condition is violated, thus implying our claim. Indeed, $\mathbb{P}_{x_0,0}^1(\sigma_t = 1)$ can be bounded from below by the probability that the process makes only one chemical jump in the time interval $[0, t]$. Therefore, taking $x_0 < t$, we get

$$\begin{aligned} \mathbb{P}_{x_0,0}^1(\sigma_t = 1) &\geq \int_0^{x_0} \gamma(0|x_0 - s) e^{-\int_0^s \gamma(0|x_0 - u) du - \int_s^t \gamma(1|x_0 - s + v - s) dv} ds = \\ &\int_0^{x_0} (x_0 - s)^{-1} e^{-\int_0^s (x_0 - u)^{-1} du - \int_s^t (1 - x_0 + 2s - v)^{-1} dv} ds = \\ &x_0^{-1} \int_0^{x_0} \frac{1 - x_0 + 2s - t}{1 - x_0 + s} ds \geq x_0^{-1} \int_0^{x_0} (1 - x_0 + 2s - t) ds = 1 - t. \end{aligned} \quad (\text{B.2})$$

Therefore, the supremum over $x_0 \in (0, 1)$ in the l.h.s. of (B.1) is at least $(1 - t)/t$. This implies that (B.1) is violated.

Finally, we come back to the observations about the existence of the invariant measure collected in Section 3. We take (x_0, σ_0) as initial state and write ν_t for the distribution at time t . By compactness arguments, we know that the sequence of probability measures $\tilde{\nu}_t := t^{-1} \int_0^t \nu_s ds$ admits a subsequence weakly converging to a probability measure ν_* on the closure $\bar{\Omega} \times \Gamma$. Let us show that ν_* has support on $\Omega \times \Gamma$, thus implying that ν_* describes a steady state of the PDMP. Consider the interval $I_\varepsilon = (0, \varepsilon)$, $\varepsilon < 1$. When the mechanical state enters in the interval I_ε , the chemical state of the system must be 0. After a time of order $O(\varepsilon)$ the system jumps into the chemical state 1 keeping this value for a time $O(1)$. During this interval $x(t)$ moves on the right with constant velocity, spending at most $O(\varepsilon)$ time inside I_ε . Hence, in a time interval of order $O(1)$ the mechanical state is in I_ε for at most $O(\varepsilon)$ time. This implies that $\tilde{\nu}_t(I_\varepsilon \times \Gamma) \leq c\varepsilon$, for each t . It is simple to conclude that the limiting measure ν_* must give zero weight to $\{0\} \times \Gamma$. The same conclusion holds for the set $\{1\} \times \Gamma$, thus proving that $\nu_*(\{0, 1\} \times \Gamma) = 0$.

APPENDIX C. AN EXAMPLE OF 1D PDMP WITH A FINITE NUMBER OF JUMPS

We take here $\Omega = [0, 1]$ and $\Gamma = \{0, 1\}$. The vector fields are given by $F_0(x) = -x$ and $F_1(x) = 1 - x$ and the jump rates by $r(0, 1|x) = x$ and $r(1, 0|x) = 1 - x$.

Let us consider the process with initial condition given by $(x^*, 0)$, with x^* a generic element of Ω . We can easily compute the probability that there are no chemical jumps

$$\mathbb{P}_{(x^*, 0)}^\lambda(\sigma(t) = 0, \forall t \in \mathbb{R}^+) = e^{-\lambda x^* \int_0^{+\infty} e^{-t} dt} = e^{-\lambda x^*} \geq e^{-\lambda}. \quad (\text{C.1})$$

A similar estimate can be obtained also if we consider the process starting from the chemical state 1. The above result (C.1) states that every time the process jumps into a new chemical state σ , with positive probability uniformly bounded from below by $e^{-\lambda}$ it will never more change its chemical state and consequently the mechanical variable will definitely evolve according to the ODE $\dot{x} = F_\sigma(x)$. As a consequence it is easy to derive that this PDMP has a.s. a finite number of jumps and that the invariant measures are of the form

$$c\delta(x)\delta_{\sigma,0} + (1 - c)\delta(x - 1)\delta_{\sigma,1}, \quad c \in [0, 1].$$

APPENDIX D. DERIVATION OF (7.20) IN THE GENERAL CASE

We consider here the case that there exists some $\sigma \in \Gamma$ for which $\chi_\sigma = 0$. For simplicity we assume $\chi_{\sigma_1} = 0$ and $\chi_\sigma > 0$ for any $\sigma \neq \sigma_1$. The general case can be proved in the same way. Let us define $\Gamma^1 := \{\sigma \in \Gamma : \sigma \neq \sigma_1\}$ and $W^1 := \{(\sigma, \sigma') \in W : \sigma \neq \sigma_1, \sigma' \neq \sigma_1\}$. We want to show that

$$\inf_{z \in (0, +\infty)^\Gamma} \sum_{(\sigma, \sigma') \in W} \chi_\sigma r(\sigma, \sigma'|x) \frac{z_{\sigma'}}{z_\sigma} = \inf_{z \in (0, +\infty)^{\Gamma^1}} \sum_{(\sigma, \sigma') \in W^1} \chi_\sigma r(\sigma, \sigma'|x) \frac{z_{\sigma'}}{z_\sigma}. \quad (\text{D.1})$$

The r.h.s. of (D.1) is clearly less or equal than the l.h.s. To prove the opposite inequality take $z \in (0, +\infty)^{\Gamma^1}$ and consider $z^\epsilon := (\epsilon, z) \in (0, +\infty)^\Gamma$. We have that

$$\lim_{\epsilon \rightarrow 0} \sum_{(\sigma, \sigma') \in W} \chi_\sigma r(\sigma, \sigma'|x) \frac{z_{\sigma'}^\epsilon}{z_\sigma^\epsilon} = \sum_{(\sigma, \sigma') \in W^1} \chi_\sigma r(\sigma, \sigma'|x) \frac{z_{\sigma'}}{z_\sigma},$$

and this implies (D.1). This argument shows that we can write (7.21) and (7.22) as

$$j(x, \chi) = \sum_{\sigma} \chi_{\sigma} \gamma(\sigma|x) - \inf_{z \in (0, +\infty)^{\Gamma^1}} \sum_{(\sigma, \sigma') \in W^1} \chi_{\sigma'} r(\sigma, \sigma'|x) \frac{z_{\sigma'}}{z_{\sigma}}, \quad (\text{D.2})$$

$$j^+(x, \chi) = \sum_{\sigma} \chi_{\sigma} \gamma^+(\sigma|x) - \inf_{z \in (0, +\infty)^{\Gamma^1}} \sum_{(\sigma, \sigma') \in W^1} \chi_{\sigma'} r(\sigma, \sigma'|x) \frac{\rho(x, \sigma) z_{\sigma}}{\rho(x, \sigma') z_{\sigma'}}. \quad (\text{D.3})$$

If we introduce $\tilde{z}_{\sigma} := \frac{\chi_{\sigma}}{\rho(x, \sigma) z_{\sigma}}$ for any $\sigma \in \Gamma^1$ the variational expression in (D.3) can be written as

$$\inf_{z \in (0, +\infty)^{\Gamma^1}} \sum_{(\sigma, \sigma') \in W^1} \chi_{\sigma'} r(\sigma, \sigma'|x) \frac{\tilde{z}_{\sigma'}}{\tilde{z}_{\sigma}},$$

which coincides with the variational expression in (D.2). Relation (7.20) now follows directly.

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